



Supplement of

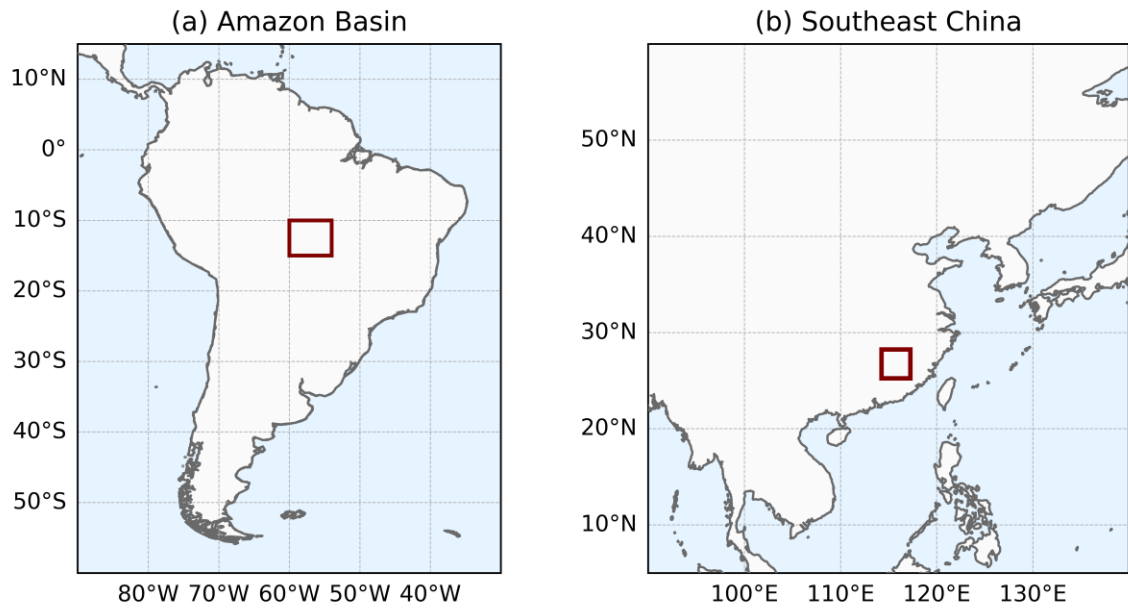
Benchmarking conditioners in Liang–Kleeman Information Flow: application to land–atmosphere interactions in humid forests

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Supplementary Figures S1–S13, Supplementary Tables S1–S3, and Supplementary Note S1 support the Information Flow analysis presented in the main manuscript.



Supplementary Fig. S1. Location of the two humid-forest study regions. (a) Amazon Basin (54–60°W, 10–15°S) and (b) Southeast China (114.25–117.25°E, 25.25–28.25°N).

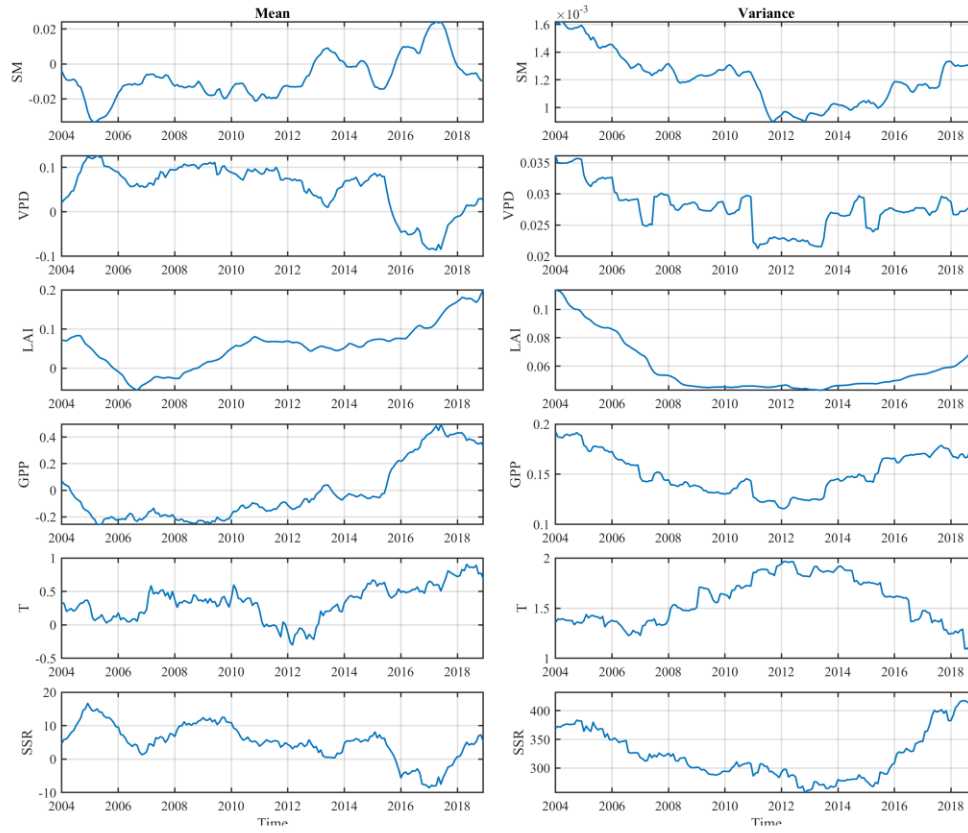
Supplementary Table S1. Statistical significance of the SM→GPP IF in Southeast China under progressive conditioning. Significant months are reported as counts and percentages out of the 180-month analysis period. Mean IF (nats/month) is calculated only over months in which the corresponding IF estimate is statistically significant.

SM→GPP IF	Number of significant months	Percentage of significant months (%)	Mean IF over significant months (nats/month)
Bivariate	13/180	7.2%	0.0352
Conditioned on VPD	116/180	64.4%	0.0461
Conditioned on VPD + T	105/180	58.3%	0.0472
Conditioned on VPD + SSR	115/180	63.9%	0.0456
Conditioned on VPD + T + SSR	105/180	58.3%	0.0466

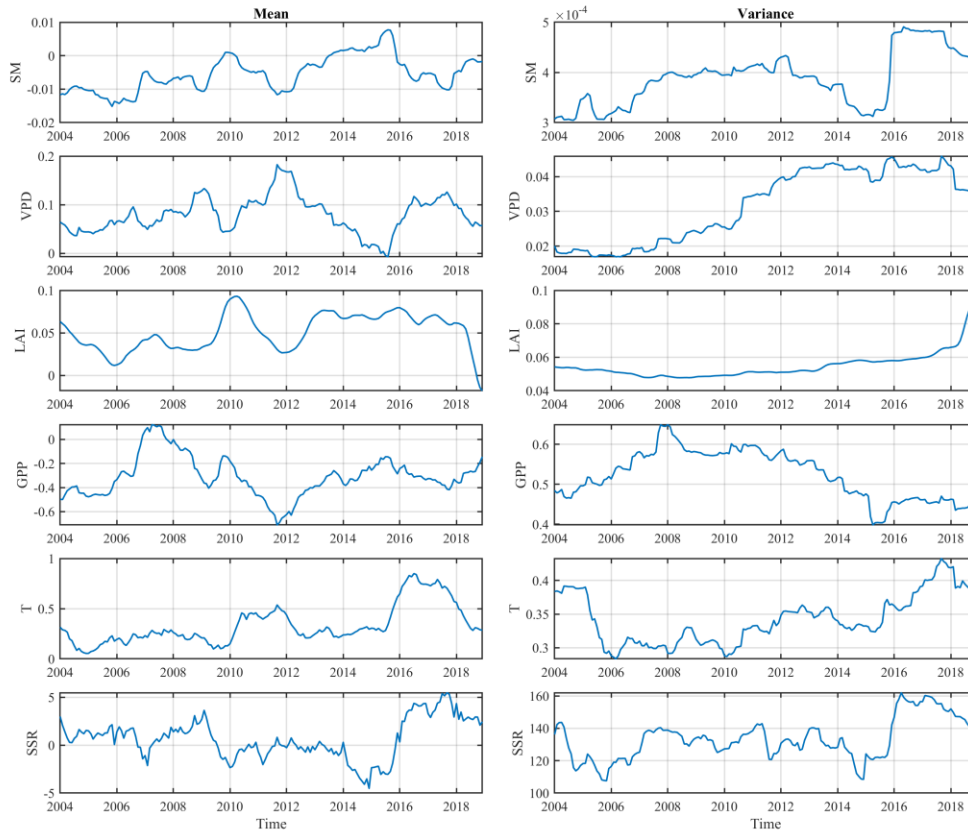
Supplementary Table S2. Statistical significance of the SM→GPP IF in the Amazon Basin under progressive conditioning. Significant months are reported as counts and percentages out of the 180-month analysis period. Mean IF (nats/month) is calculated only over months in which the corresponding IF estimate is statistically significant.

SM→GPP IF	Number of significant months	Percentage of significant months (%)	Mean IF over significant months (nats/month)
Bivariate	73/180	40.6%	-0.0225
Conditioned on VPD	50/180	27.8%	0.0175
Conditioned on VPD + T	43/180	23.9%	0.0224
Conditioned on VPD + SSR	54/180	30.0%	0.0124
Conditioned on VPD + T + SSR	41/180	22.8%	0.0205

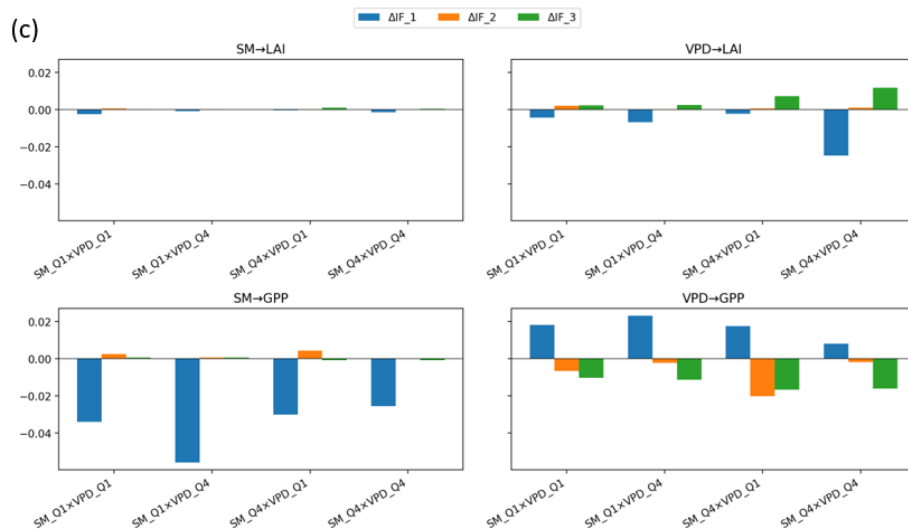
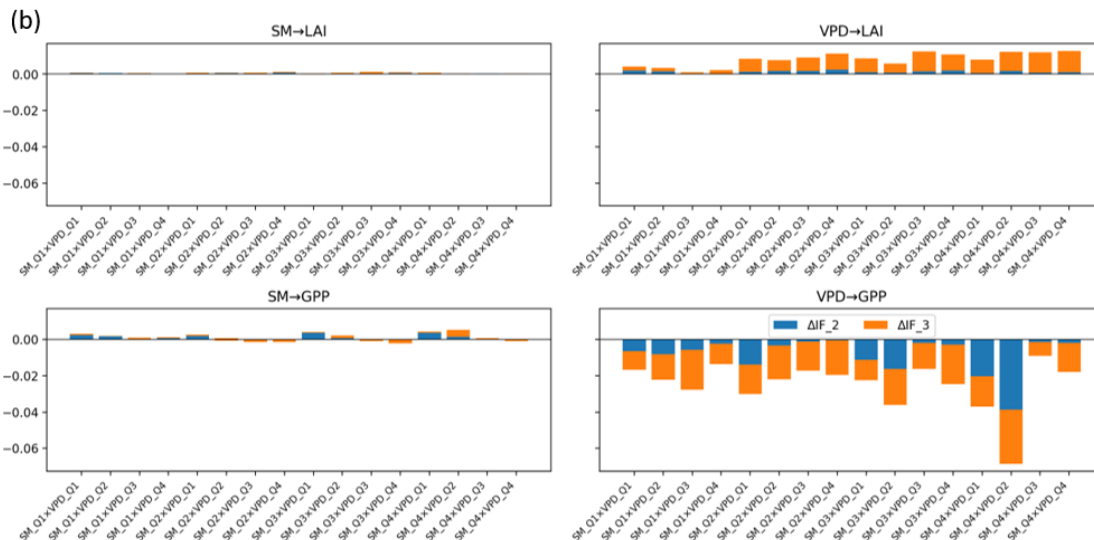
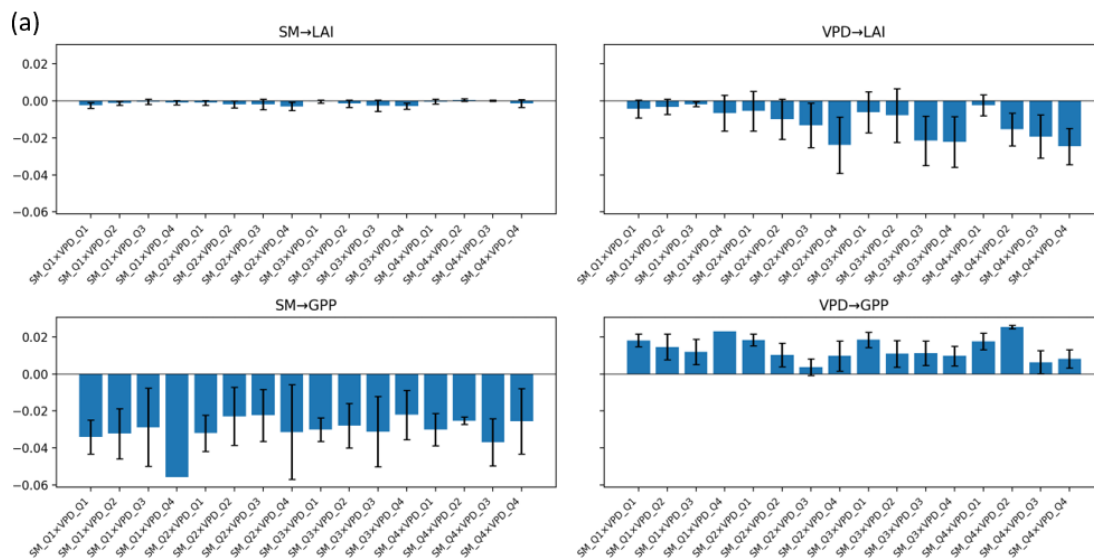
(a) Southeast China



(b) Amazon Basin



Supplementary Fig. S2. Temporal evolution of the means (left column) and variances (right column) of SM, VPD, LAI, GPP, T, and SSR for (a) Southeast China and (b) the Amazon Basin during 2004–2018. The statistics were calculated from the same anomaly time series and using the same temporal settings as in the LKIF analysis (Materials and Methods). The units of the mean time series are $\text{m}^3 \text{m}^{-3}$ for SM, kPa for VPD, $\text{m}^2 \text{m}^{-2}$ for LAI, $\text{g C m}^{-2} \text{d}^{-1}$ for GPP, $^{\circ}\text{C}$ for T, and W m^{-2} for SSR. The variances are expressed in the corresponding squared units.



Supplementary Fig. S3. Δ Information Flow (Δ IF) for SM $\rightarrow$ LAI, VPD $\rightarrow$ LAI, SM $\rightarrow$ GPP, and VPD $\rightarrow$ GPP across combined quartiles of soil moisture (SM) and vapor pressure deficit (VPD) for southeast China. Each panel illustrates how Δ IF varies across environmental regimes defined by water supply (SM: Q1–Q4) and atmospheric demand (VPD: Q1–Q4), shown for three conditioning levels.

(a) Δ IF_1, computed as the difference between the bivariate IF and the IF conditioned only on the paired driver (i.e., SM conditioned on VPD, or VPD conditioned on SM).

(b) Δ IF_2 and Δ IF_3, computed as the difference between the bivariate IF and the IF conditioned on the paired driver and temperature (SM/VPD and T/R, respectively).

(c) Δ IF_1, Δ IF_2 and Δ IF_3 represent the differences between the bivariate IF and the multivariate IF under three conditioning schemes.

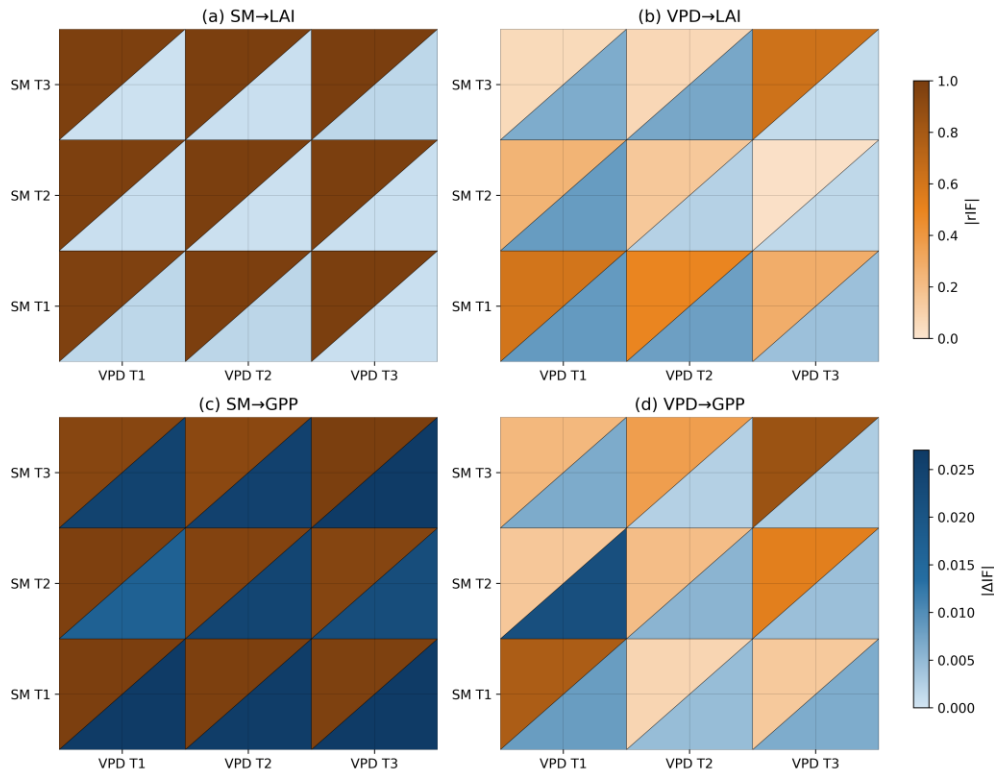
Δ IF_1: SM $\rightarrow$ LAI/GPP conditioned on VPD, and VPD $\rightarrow$ LAI/GPP conditioned on SM;

Δ IF_2: SM $\rightarrow$ LAI/GPP or VPD $\rightarrow$ LAI/GPP conditioned on the paired driver and temperature (SM/VPD + T);

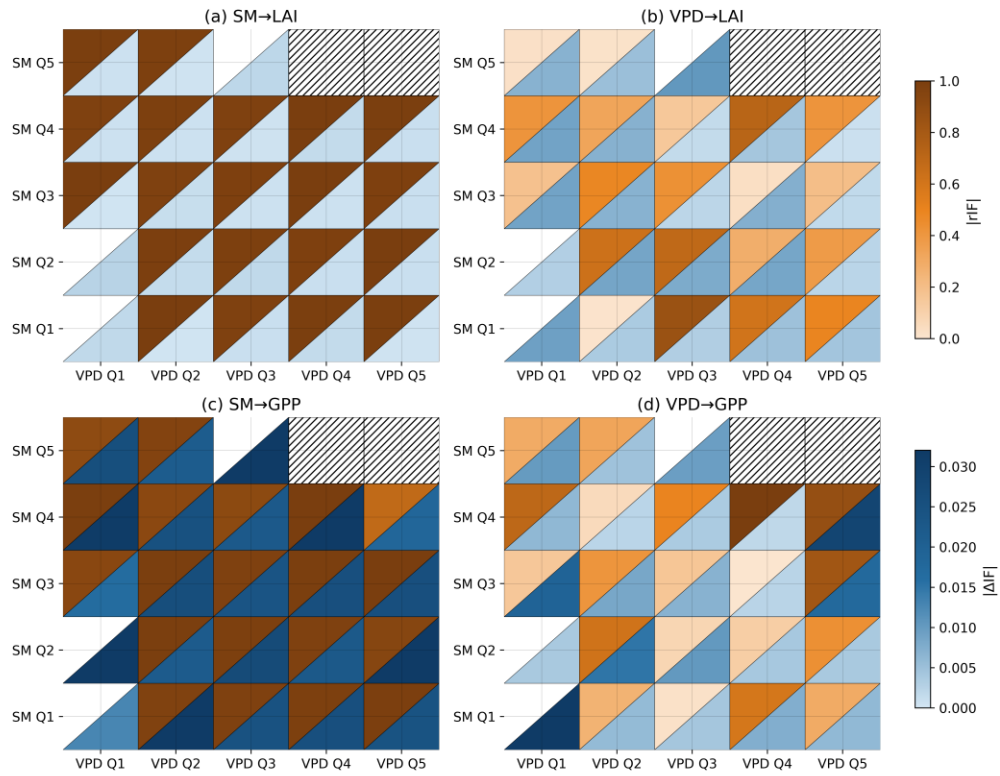
Δ IF_3: SM $\rightarrow$ LAI/GPP or VPD $\rightarrow$ LAI/GPP conditioned on the paired driver, temperature, and surface solar radiation (SM/VPD + T + SSR).

Across all panels, bar heights indicate the magnitude of Δ IF for each SM–VPD quartile combination, with error bars showing the 95% confidence interval. These supplementary plots provide a detailed view of how Δ IF responds to changing hydroclimatic conditions and conditioner configurations, complementing the combined rIF– Δ IF diagnostic presented in Figure 3.

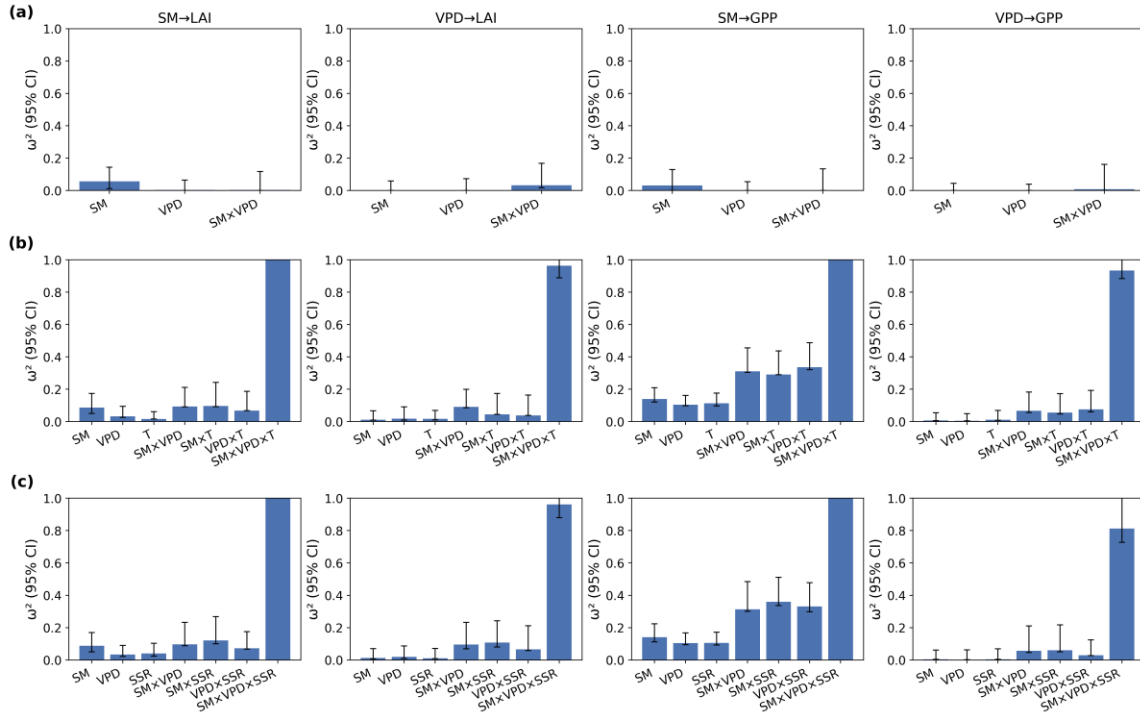
State-Dependent patterns of changes in information flow – Using Terciles



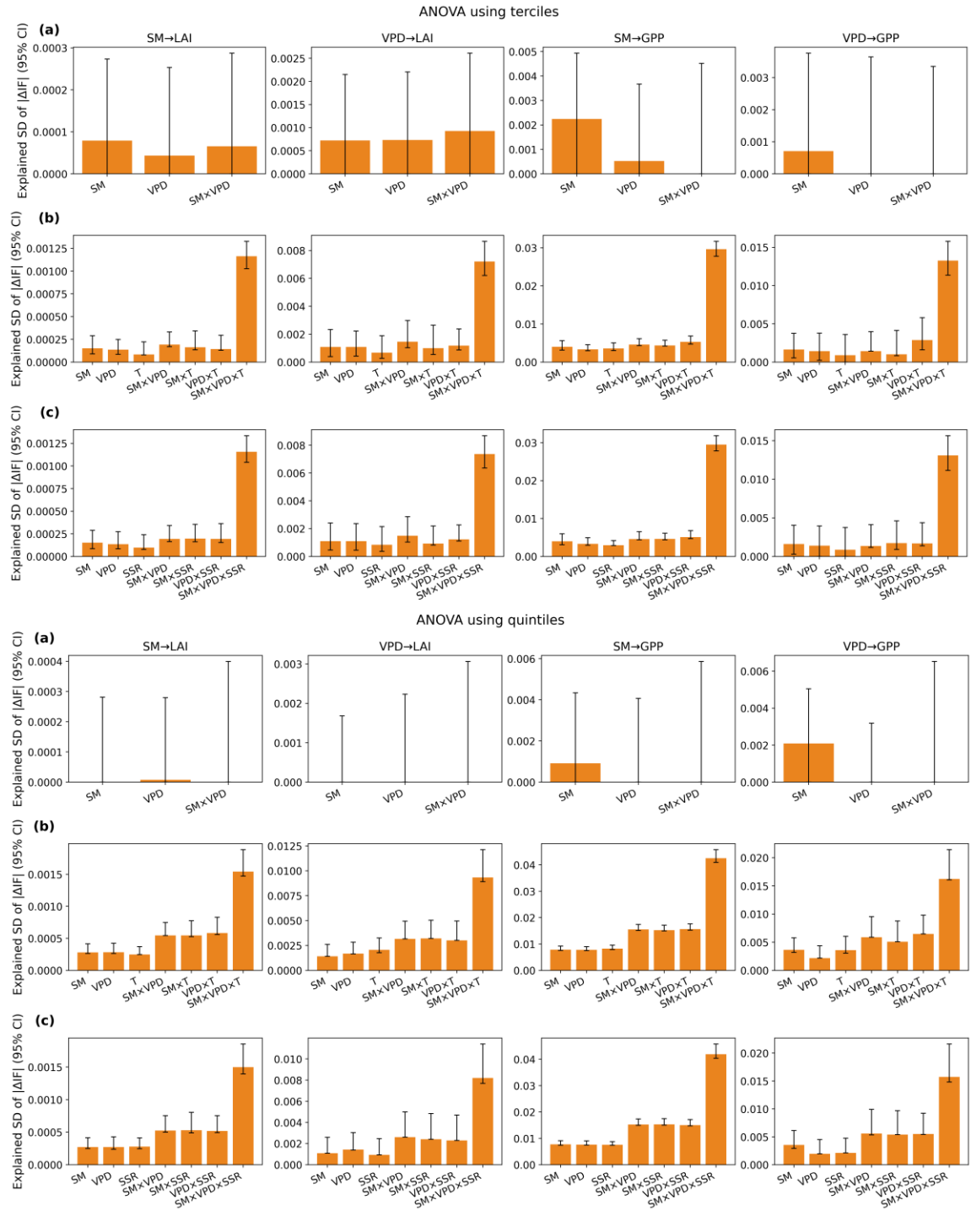
State-Dependent patterns of changes in information flow – Using Quintiles



Supplementary Fig. S4. Differences (Δ IF) and correlations (rIF) between bivariate and multivariate Information Flow across SM and VPD terciles (Q1–Q3; top panel) and quintiles (Q1–Q5; bottom panel) for Southeast China. (a) SM→LAI, (b) VPD→LAI, (c) SM→GPP, and (d) VPD→GPP. Each cell is divided into an upper triangle ($|rIF|$: magnitude of Pearson correlation between bivariate and multivariate IF) and a lower triangle ($|\Delta IF|$: absolute difference between bivariate and multivariate IF). Colour intensities are scaled independently for each triangle using separable colormaps. Blank upper triangles, such as that for SM(Q1)–VPD(Q1), indicate SM–VPD regime combinations for which only two paired observations ($n=2$) were available; in these cases, $|rIF|$ was not reported because Pearson correlation is not statistically informative with $n=2$, while the corresponding $|\Delta IF|$ value was retained. Cross-hatched cells indicate combinations with no data. (SM= Soil Moisture, VPD= Vapor Pressure Deficit, LAI= Leaf Area Index, GPP= Gross Primary Productivity).

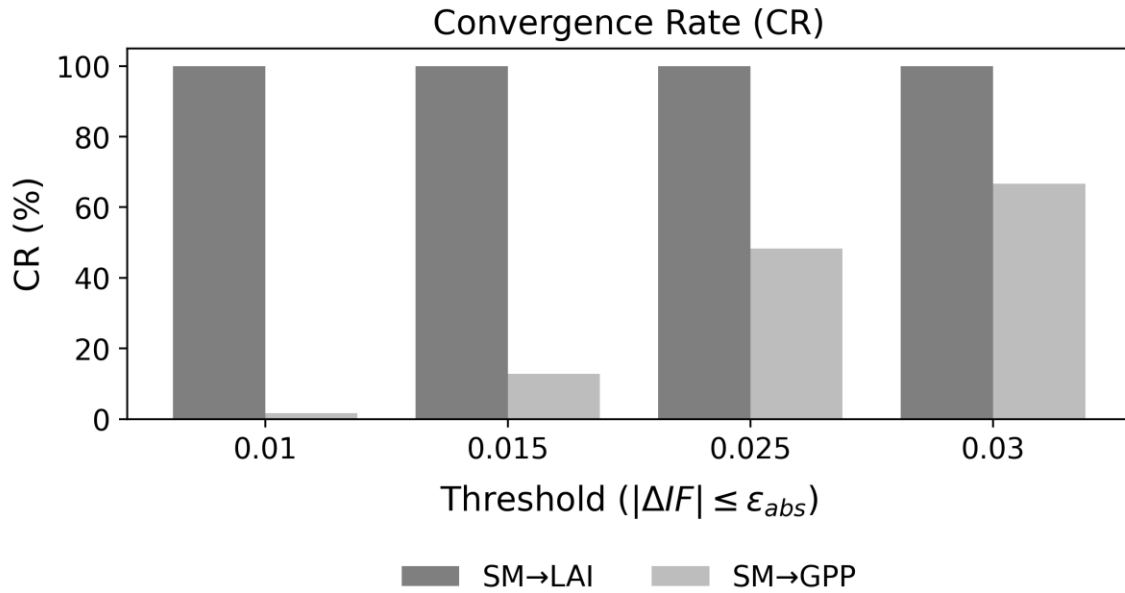


Supplementary Fig. S5. Fraction of variance (ω^2) for $|\Delta IF|$ attributed to each ANOVA factor and interaction, corresponding to the same regime structures used in Fig. 4. Bars show the relative dominance of soil moisture (SM), vapor pressure deficit (VPD), temperature (T), surface solar radiation (SSR), and their interactions in explaining variability in $|\Delta IF|$ across pathways.

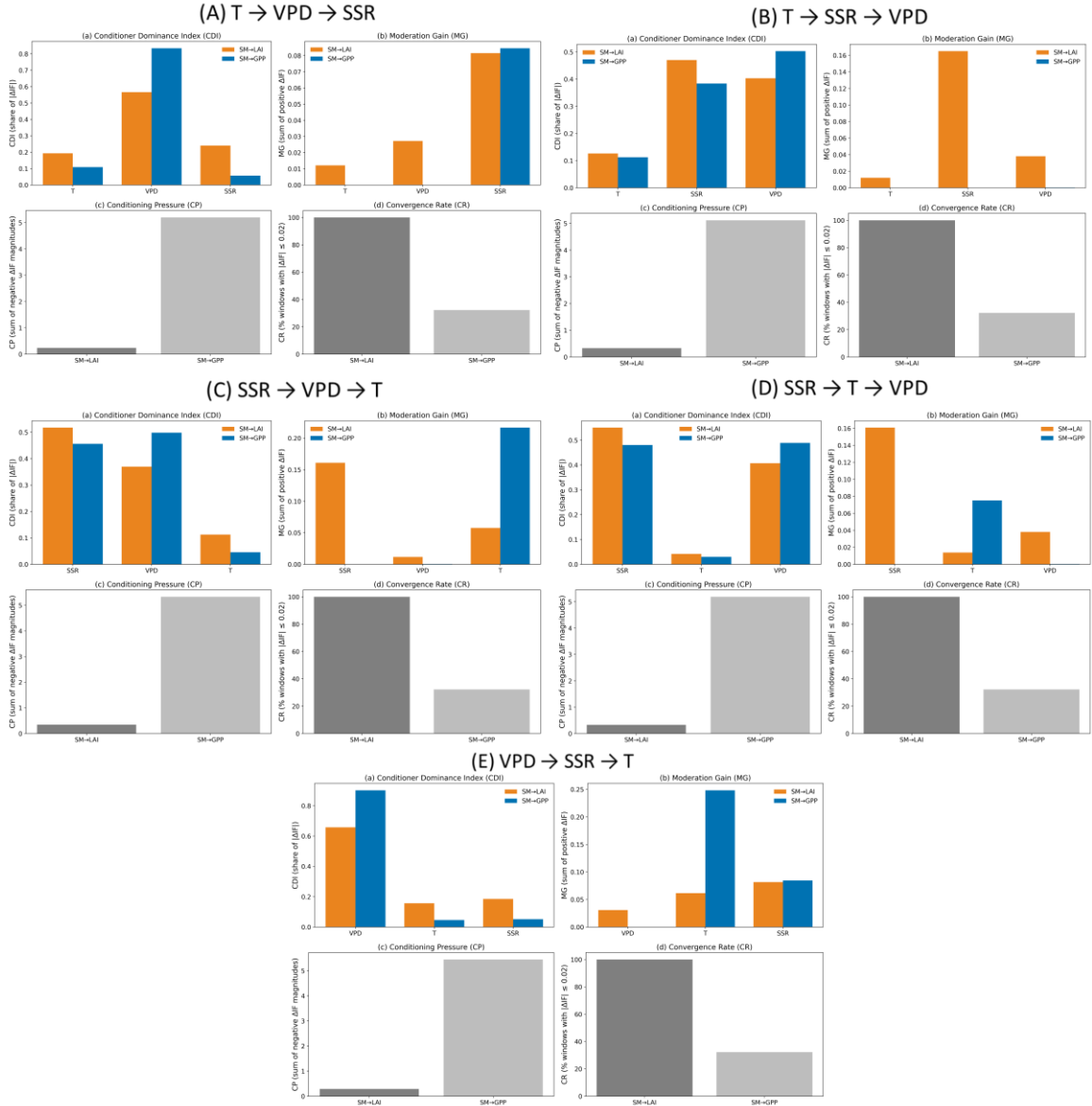


Supplementary Fig. S6. Sensitivity of the ANOVA decomposition to the number of quantile bins: terciles (top panel) and quintiles (bottom panel). ANOVA results showing the explained standard deviation ($\sqrt{\Delta EV}$)

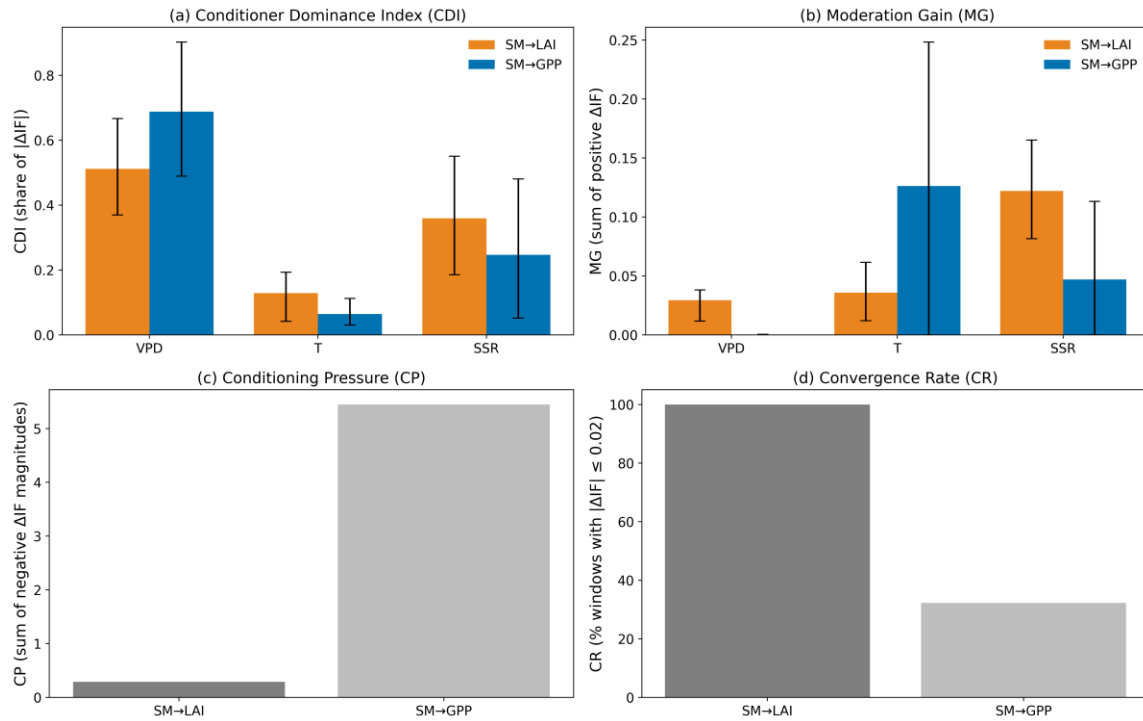
of $|\Delta IF|$ for Southeast China. Columns represent the four pathways: SM→LAI, VPD→LAI, SM→GPP, and VPD→GPP. (a) Two-way ANOVA with factors SM and VPD. (b) Three-way ANOVA including SM, VPD, and T. (c) Three-way ANOVA including SM, VPD, and SSR. Bars show the explained SD for each factor or factor interaction; error bars indicate the 95% confidence interval. (SM= Soil Moisture, VPD= Vapor Pressure Deficit, T= Temperature, SSR= Surface Solar Radiation). Note that the Y-axis range differs in each panel to better see the different values.



Supplementary Fig. S7. Convergence Rate (CR) to the absolute divergence threshold ϵ_{abs} for the Southeast China SM→LAI and SM→GPP couplings. CR was recalculated using $\epsilon_{abs} = 0.01, 0.015, 0.025$, and 0.03 . SM→LAI remains consistently near full convergence across all tested thresholds, whereas SM→GPP shows strong threshold dependence, although it remains substantially less convergent than SM→LAI.

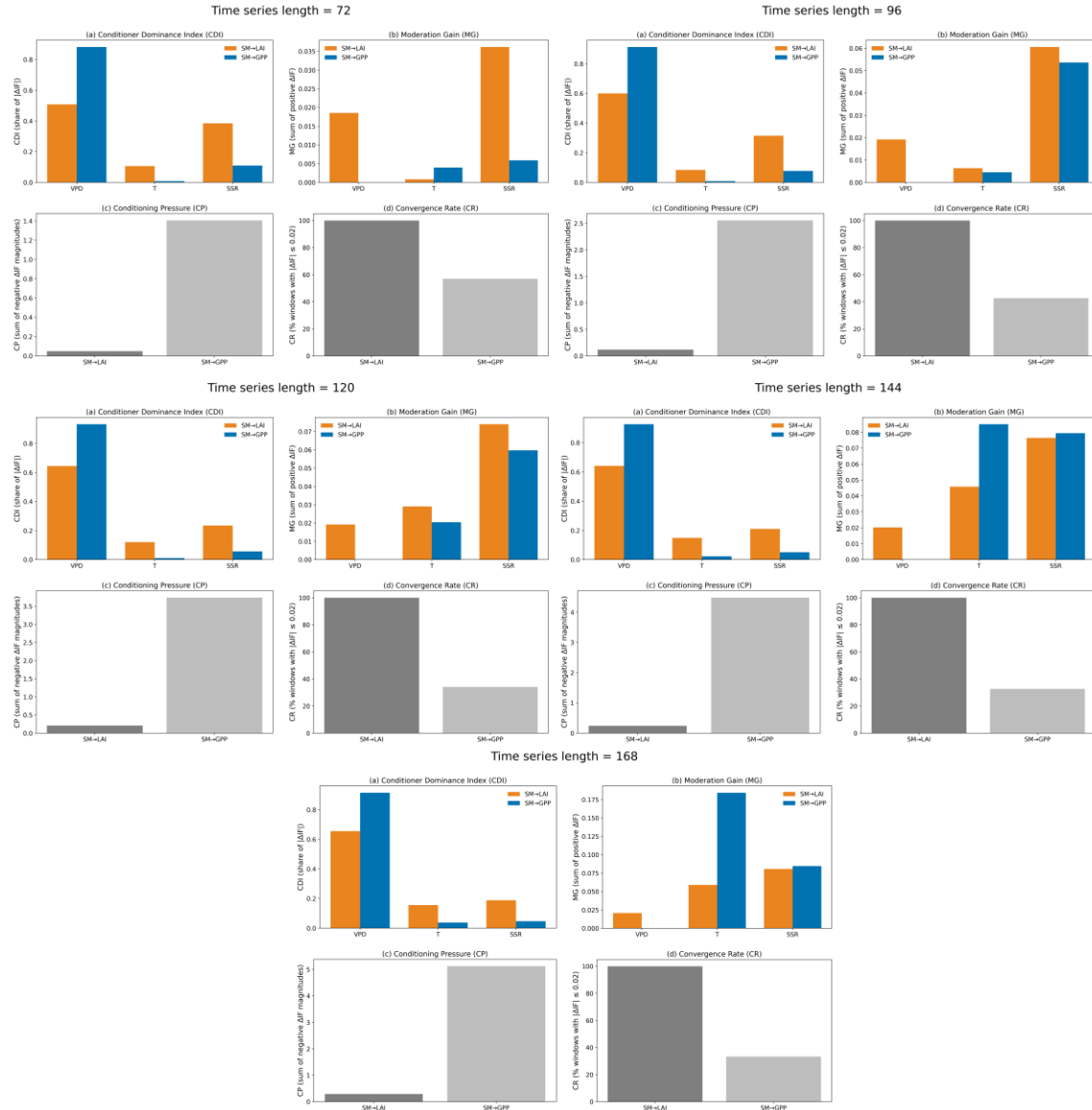


Supplementary Fig. S8. Sensitivity of decomposition indices to conditioner ordering. CDI, MG, CP, and CR are computed for different permutations of the conditioning variables (VPD, T, SSR). Panels (A–E) represent alternative ordering sequences: (A) $T \rightarrow VPD \rightarrow SSR$, (B) $T \rightarrow SSR \rightarrow VPD$, (C) $SSR \rightarrow VPD \rightarrow T$, (D) $SSR \rightarrow T \rightarrow VPD$, and (E) $VPD \rightarrow SSR \rightarrow T$. CDI and MG vary with permutation order, indicating order dependence, whereas CR remains invariant and the aggregated CP remains unchanged in this application. Results are shown for both SM–LAI and SM–GPP pathways. CP is shown as the accumulated value across conditioners for each pathway.



Supplementary Fig. S9. Robustness of four diagnostic indices to conditioner ordering.

Mean values and permutation ranges of CDI, MG, CP, and CR were calculated across all possible ordering sequences of the conditioning variables (VPD, T, and SSR). Bars denote the mean across permutations and error bars indicate the corresponding range. Results are shown for both SM→LAI and SM→GPP pathways. In panel (c), CP is shown as the accumulated value across conditioners for each pathway.



Supplementary Fig. S10. Sensitivity of CDI, MG, CP, and CR to time-series length. The indices were recomputed using records of 72, 96, 120, 144, and 168 months. While MG and CP show dependence on record length due to their cumulative definitions, the CDI and CR remain consistent across all lengths for both SM→LAI and SM→GPP. CP is shown as the accumulated value across conditioners for each pathway.

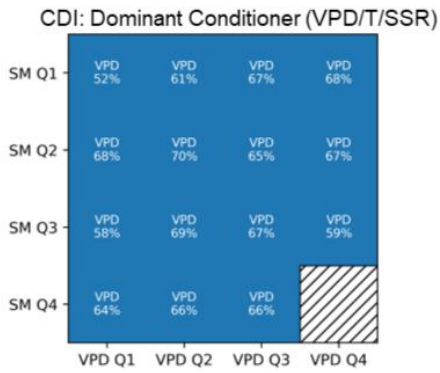
Sensitivity to record length was evaluated by recomputing the indices using truncated time series (72–168 months). The dominant conditioner identified by CDI remained consistent across all lengths, while MG and CP exhibited length dependence consistent with their cumulative definitions. CR remained persistently high for SM→LAI and substantially lower for SM→GPP across all lengths, indicating that pathway-level contrasts are stable with respect to sampling length.

Supplementary Table S3. Sensitivity of CDI, MG, CP, and CR to Gaussian noise of the stepwise $\Delta I F$ series.
Values are reported as mean $\pm$ standard deviation across 200 realizations for noise levels corresponding to 5%, 10%, and 20% of the standard deviation of each series.

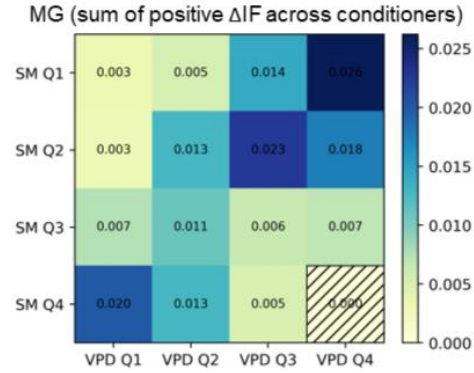
Couplings	Noise (%)	CDI_VPD	CDI_T	CDI_SSR	MG_VPD	MG_T	MG_SSR	CP	CR (%)
SM→GPP	5	0.9016 $\pm$ 0.0003	0.0466 $\pm$ 0.0002	0.0518 $\pm$ 0.0002	0.0 $\pm$ 0.0	0.2493 $\pm$ 0.0011	0.0849 $\pm$ 0.0008	5.4478 $\pm$ 0.0108	32.0389 $\pm$ 1.0525
SM→GPP	10	0.9008 $\pm$ 0.0006	0.0473 $\pm$ 0.0004	0.052 $\pm$ 0.0004	0.0 $\pm$ 0.0	0.2514 $\pm$ 0.0021	0.0855 $\pm$ 0.0017	5.4512 $\pm$ 0.0197	31.9111 $\pm$ 1.261
SM→GPP	20	0.8981 $\pm$ 0.0013	0.0493 $\pm$ 0.0008	0.0526 $\pm$ 0.0009	0.0001 $\pm$ 0.0004	0.2577 $\pm$ 0.0041	0.0874 $\pm$ 0.0034	5.4602 $\pm$ 0.0409	31.4583 $\pm$ 1.7341
SM→LAI	5	0.6574 $\pm$ 0.0013	0.1566 $\pm$ 0.0008	0.186 $\pm$ 0.0009	0.0308 $\pm$ 0.0006	0.0615 $\pm$ 0.0003	0.0817 $\pm$ 0.0004	0.2903 $\pm$ 0.0012	100.0 $\pm$ 0.0
SM→LAI	10	0.6567 $\pm$ 0.0023	0.1564 $\pm$ 0.0014	0.1868 $\pm$ 0.0017	0.0314 $\pm$ 0.0013	0.0617 $\pm$ 0.0005	0.0821 $\pm$ 0.0007	0.2914 $\pm$ 0.0023	100.0 $\pm$ 0.0
SM→LAI	20	0.6543 $\pm$ 0.0043	0.1566 $\pm$ 0.0027	0.1891 $\pm$ 0.0033	0.0337 $\pm$ 0.0025	0.0623 $\pm$ 0.001	0.0834 $\pm$ 0.0014	0.2958 $\pm$ 0.004	100.0 $\pm$ 0.0

SM→LAI: Indices across SM×VPD quartiles

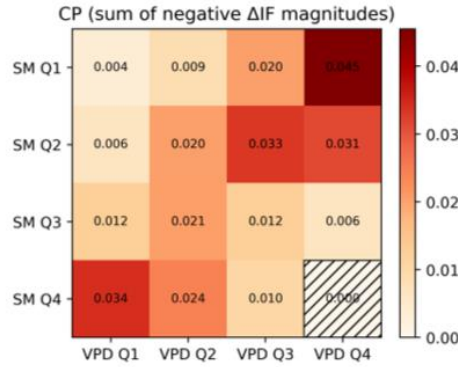
(a)



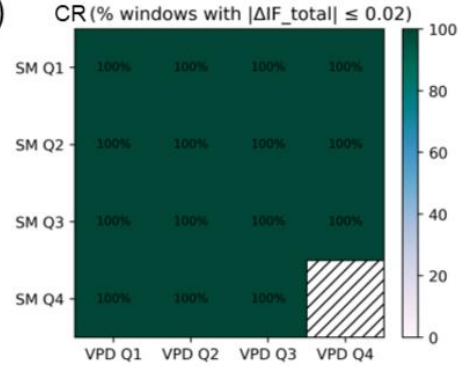
(b)



(c)

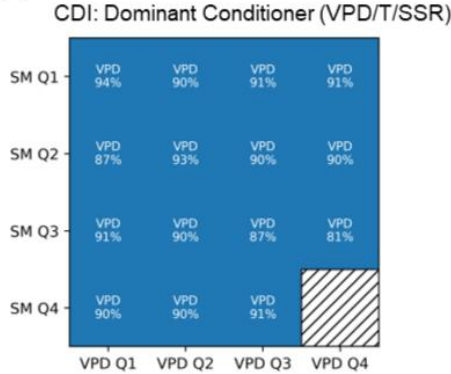


(d)

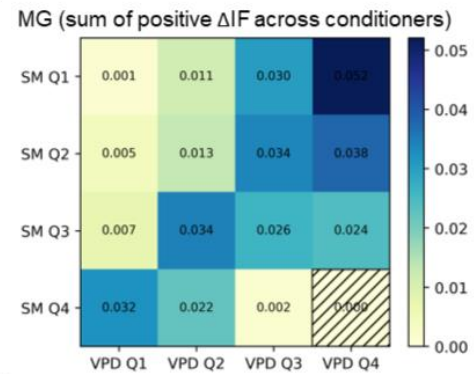


SM→GPP: Indices across SM×VPD quartiles

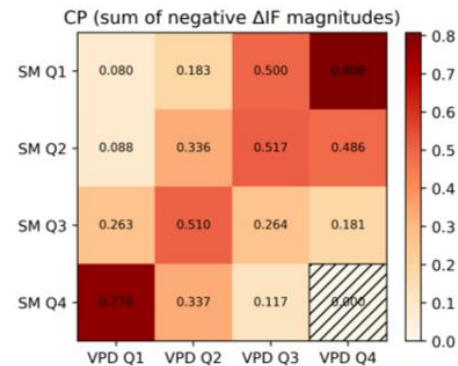
(a)



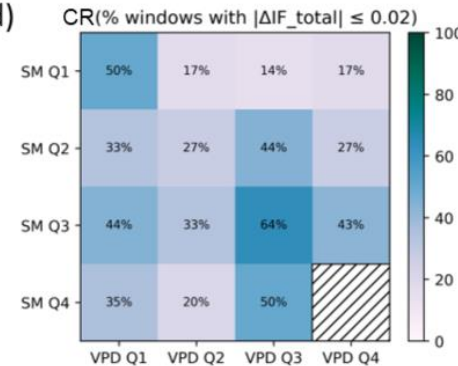
(b)



(c)

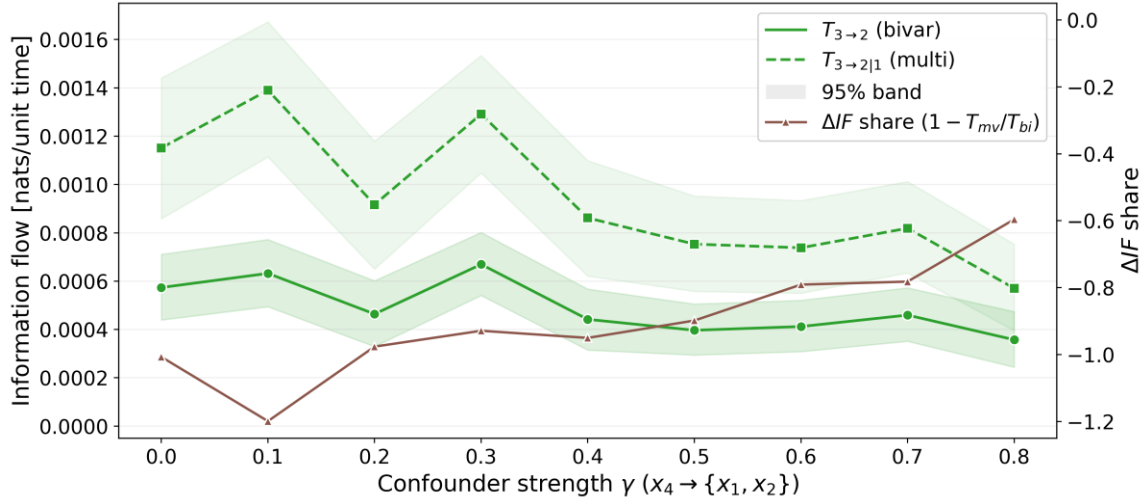


(d)



Supplementary Fig. S11. Conditioner-decomposition indices (a: Conditioner Dominance Index; b: Moderation Gain; c: Conditioning Pressure; d: Convergence Rate) evaluated separately across all SM–VPD quartile regimes for the SM→LAI and SM→GPP pathways.

These panels complement Fig. 5 by illustrating how the importance of conditioners varies across distinct hydroclimatic conditions.



Supplementary Fig. S12. Synthetic LKIF experiment illustrating enhancement of information flow after conditioning. The VAR (1) configuration is identical to that used in Appendix A except that the $x_1 \rightarrow x_2$ coefficient is reversed from $C_{12}=0.45$ to $C_{12}=-0.45$, causing the direct $x_3 \rightarrow x_2$ pathway and the indirect pathway through x_1 to act in opposite directions. The conditioned $T_{3 \rightarrow 2|1}$ exceeds the corresponding bivariate $T_{3 \rightarrow 2}$ throughout the tested confounder-strength range. The brown line shows the normalized difference (right y-axis). The shaded band shows the 95% confidence intervals.

S1: Synthetic data experiment

To complement the hidden-confounder experiment presented in Appendix A, we perform an additional controlled synthetic experiment designed specifically to determine whether a prescribed direct source-to-target coupling can appear weak or statistically non-significant in a bivariate formulation but remain detectable when an observed common driver is included as a conditioner, as in our real-world case study (Fig. 1c). The experiment uses a three-dimensional, linear, stable first-order Vector Autoregressive (VAR1) process defined as (Eq. S1);

$$\mathbf{x}_t = A\mathbf{x}_{t-1} + \boldsymbol{\varepsilon}_t, \quad \boldsymbol{\varepsilon}_t \sim \mathcal{N}(0, \Sigma), \quad (\text{S1})$$

where $\mathbf{x}_t = (x_{1,t}, x_{2,t}, x_{3,t})^\top$ are the three different time series and $\Sigma = \text{diag}(b_1^2, b_2^2, b_3^2)$, with b_i being the stochastic perturbation amplitudes. The coefficient matrix A is (Eq. S2);

$$A = \begin{pmatrix} \phi & c_{21} & c_{31} \\ c_{12} & \phi & c_{32} \\ 0 & 0 & \phi \end{pmatrix} \quad (\text{S2})$$

where $\phi = 0.44$, $c_{21} = 0.15$, $c_{31} = 0.25$, and $c_{12} = 0.30$ are held fixed, whereas c_{32} is varied. The innovation scales are $(b_1, b_2, b_3) = (0.35, 1.15, 0.53)$. The fixed coefficients are assigned different magnitudes because the pathways play different dynamical roles. The direct $x_1 \rightarrow x_2$ pathway is the strongest fixed cross-variable coupling, the $x_3 \rightarrow x_1$ common-driver pathway is intermediate, and the $x_2 \rightarrow x_1$ feedback is weaker. These parameter values were chosen to define a stable asymmetric synthetic system for the controlled experiment and were not estimated from the observational data. Expanding the (VAR1) system by rows gives (Eq. S3);

$$\begin{aligned} x_{1,t} &= \phi x_{1,t-1} + c_{21} x_{2,t-1} + c_{31} x_{3,t-1} + \varepsilon_{1,t}, \\ x_{2,t} &= \phi x_{2,t-1} + c_{12} x_{1,t-1} + c_{32} x_{3,t-1} + \varepsilon_{2,t}, \\ x_{3,t} &= \phi x_{3,t-1} + \varepsilon_{3,t}. \end{aligned} \quad (\text{S3})$$

The causal structure contains a bidirectional interaction between x_1 and x_2 together with unidirectional influences $x_3 \rightarrow x_1$ and $x_3 \rightarrow x_2$. As c_{32} departs from zero, x_3 acts as an observed common driver because it influences both the source x_1 and the target x_2 . In contrast, c_{32} is assigned the opposite sign to the $x_1 \rightarrow x_2$ pathway and is progressively strengthened. To sample this transition systematically, $|c_{32}|$ is varied uniformly from 0.0 to 2.3 in increments of 0.1 (equivalently, $c_{32} = 0, -0.1, \dots, -2.3$). For presentation, the horizontal axis is expressed as the magnitude of $x_3 \rightarrow x_2$ coupling, $|c_{32}|$. Importantly, the prescribed direct $x_1 \rightarrow x_2$ coefficient remains unchanged throughout the experiment.

For every $|c_{32}|$ value, 80 independent realizations of length $N = 3000$ are generated after discarding a burn-in of 200 time steps. We compute the bivariate information flow $x_1 \rightarrow x_2$ using only x_1 and x_2 , and the multivariate information flow $x_1 \rightarrow x_{2|3}$ after including x_3 as the conditioning variable. To evaluate how

conditioning alters the estimated causal strength, the differential information flow is calculated using the same convention as in the main manuscript (Eq. S4),

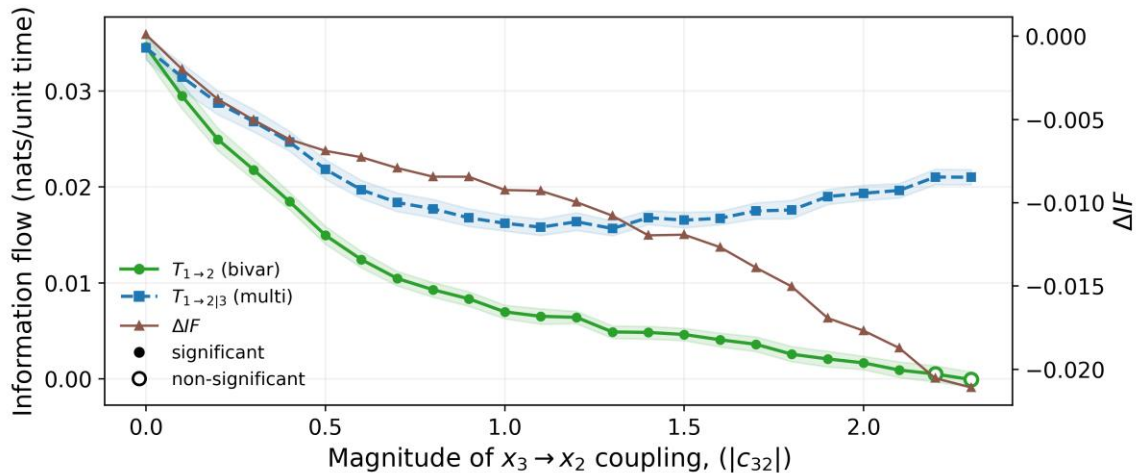
$$\Delta IF_{1 \rightarrow 2} = T_{1 \rightarrow 2}^{(bi)} - T_{1 \rightarrow 2|3}^{(mv)} \quad (S4)$$

Across the 80 realizations, the ensemble-mean information flow and its 95% percentile bootstrap confidence interval are estimated using $B=1000$ bootstrap samples. For this synthetic experiment, an ensemble-mean IF is classified as statistically significant when its 95% bootstrap confidence interval excludes zero.

The results are summarized in Supplementary Fig. S13. When $|c_{32}| = 0$, the bivariate and conditioned estimates are almost identical, indicating no effect of conditioning. As the $x_3 \rightarrow x_2$ influence becomes stronger, however, the bivariate $T_{1 \rightarrow 2}$ progressively decreases even though the prescribed direct $x_1 \rightarrow x_2$ coefficient remains fixed. $T_{1 \rightarrow 2|3}$ also decreases as $|c_{32}|$ increases until $|c_{32}| = 1$ and then it increases, but it always remains larger than the bivariate $T_{1 \rightarrow 2}$ and statistically significant throughout the tested range.

Correspondingly, ΔIF becomes increasingly negative because the conditioned estimate exceeds the bivariate estimate. The negative ΔIF therefore does not indicate a negative conditioned causal pathway. Instead, it indicates that accounting for x_3 yields a larger estimate of the $x_1 \rightarrow x_2$ information flow than is apparent in the bivariate projection.

Overall, this controlled experiment demonstrates that a fixed direct source-to-target coupling can be masked in a bivariate representation when an observed common driver influences the source and target through opposing contributions, as in our real-world case study (Fig. 1c). In this configuration, omission of x_3 progressively suppresses the estimated $x_1 \rightarrow x_2$ information flow until the bivariate estimate becomes statistically indistinguishable from zero, whereas inclusion of x_3 as a conditioner retains a significantly positive $x_1 \rightarrow x_2$ pathway. The experiment therefore provides a controlled proof of principle for a conditioning-induced transition in statistical significance. It is intended as a generic dynamical experiment rather than a representation of individual land-atmosphere variables.



Supplementary Fig. S13. Controlled synthetic experiment illustrating bivariate masking and conditioned detection of LKIF under an observed common-driver structure. The direct $x_1 \rightarrow x_2$ coupling ($c_{12} = 0.30$), the $x_3 \rightarrow x_1$ coupling ($c_{31} = 0.25$), and the $x_2 \rightarrow x_1$ feedback ($c_{21} = 0.15$) remain fixed, while the magnitude of the opposing $x_3 \rightarrow x_2$ coupling is varied uniformly from 0.0 to 2.3 in increments of 0.1. The solid green and dashed blue curves show the ensemble-mean bivariate $T_{1 \rightarrow 2}$ and conditioned $T_{1 \rightarrow 2|3}$ estimates, respectively, and the shaded regions show their 95% bootstrap intervals. Filled markers indicate statistically significant estimates, whereas empty markers indicate estimates whose 95% bootstrap intervals include zero. The brown line shows ΔIF on the right axis. At $|c_{32}| = 2.2$ and 2.3, the bivariate estimate is statistically non-significant, while the conditioned estimate remains positive and significant.