



Benchmarking Conditioners in Liang–Kleeman Information Flow: Application to Land–Atmosphere Interactions

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Abstract. The Liang–Kleeman Information Flow (LKIF) framework has been increasingly used to identify causality in Earth–system dynamics in recent years. Yet, uncertainties remain regarding how the causal graph changes when mediators and confounders (conditioners) are introduced, i.e., divergence between the bivariate and conditioned forms. A controlled synthetic experiment shows that LKIF preserves correct causal directions under hidden confounding, while differences between bivariate and multivariate estimates still occur. We characterize these differences using time–varying LKIF (Δ IF) and introduce several quantifiers, including Mediator Dominance Index, Moderation Gain, Confounding Pressure, and Convergence Rate, to evaluate the contributions of conditioners. This is illustrated in an application to soil moisture (SM) and vapor pressure deficit (VPD) couplings with vegetation (Leaf Area Index (LAI) and Gross Primary Productivity (GPP)). We find that the influence of SM on LAI remains consistently direct and stable, whereas its influence on GPP and that of VPD on vegetation exhibit substantial divergence between bivariate and multivariate estimates. This divergence peaks under compound dry–hot conditions, with VPD and temperature emerging as dominant mediators. These results demonstrate that bivariate and multivariate LKIF can yield markedly different conclusions across time and space, especially under compound environmental stress. This highlights the need for multivariate conditioning when assessing vegetation responses.

1 Introduction

Land–atmosphere interactions are essential for modulating the flow of energy, water, and carbon between the surface of the land and the atmosphere, and they are especially responsive to extreme climate events. The soil–vegetation–atmosphere coupling continuum is central to these interactions, influencing and responding to changes in environmental conditions (Piao et al., 2019; Cui et al., 2020). Extreme events, like droughts and heatwaves, disrupt these interactions by depleting soil moisture (SM) and increasing vapor pressure deficit (VPD) – two key drivers of vegetation stress (Novick et al., 2016; Liu et al., 2020;



Zhong et al., 2023). While SM regulates the quantity of water accessible for plant absorption (Sperry et al., 2017), VPD indicates the atmospheric demand for water, affecting plant transpiration and stomatal function (Zhou et al., 2019). The co-occurrence of restricted water supply and heightened evaporative demand during extreme conditions can significantly stress plants, leading to a decrease in photosynthesis and hindering growth (Green et al., 2019; Liu et al., 2020). This has significant
 40 implications for food and water security, especially in water-scarce regions. It is, therefore, vital to understand how vegetation responds to variations in SM (representing moisture supply) and VPD (representing moisture demand) during extreme events for assessing ecosystem vulnerability/resilience, and to improve the prediction of vegetation–climate feedbacks. However, accurate predictions require observing and quantifying/representing these events to better understand them unhindered by relative sensitivities in climate and weather models.

45 Most existing studies have investigated the relationships among SM, VPD, and vegetation using conventional statistical techniques such as correlation and regression (Yuan et al., 2019; Zhong et al., 2023). While these approaches can reveal co-variability, they identify symmetrical relationships that do not imply causation or directionality (Stips et al., 2016; Docquier et al., 2023). As a result, utilizing basic statistical methods makes it challenging to differentiate cause from effect. To address these limitations, several causal inference techniques, such as Granger Causality (GC) and Peter and Clark Momentary
 50 Conditional Independence (PCMCI), have been suggested to investigate complex land–atmosphere interactions (Papagiannopoulou et al., 2017; Krich et al., 2020; Dubey et al., 2023). Although these methods allow to retrieve causal relationships, they continue to encounter challenges such as inconsistent or method-dependent causal estimates, strong sensitivity to assumptions (e.g., stationarity), difficulty in representing multiscale feedbacks, and limited robustness in the presence of hidden or time-varying confounders (Docquier et al., 2024; Shao et al., 2024). Recently, the Liang–Kleeman
 55 information flow (LKIF) has surfaced as an encouraging formalism to quantify cause–effect relationships (Liang, 2013, 2014, 2016, 2021). This formalism provides a quantitative measure of causation, directly derived from first principles in contrast to IF being axiomatically proposed as an ansatz, making it well-suited for understanding directional influences in environmental systems (Liang 2016).

Originally, LKIF assumed stationarity (Liang, 2013, 2014), such that causal relationships were considered constant over time.
 60 However, in reality, interactions like vegetation–climate are fundamentally non-stationary processes, such that assuming stationarity could restrict our understanding by overlooking important temporal variations, especially when anomalous events arise. To address this issue, Hagan et al. (2019) adapted the LKIF framework to handle non–stationarity, which was further extended by Zhou et al. (2024) (Z24 hereafter), into a multivariate, non-stationary form, building on the multivariate LKIF approach by Liang (2021). Z24’s multivariate approach allows for the inclusion of mediating and/or confounding variables,
 65 providing deeper insights into causal links. Here, a variable is a mediator (M) if it lies on the causal pathway between a driver X and a response Y ($X \rightarrow M \rightarrow Y$). Conditioning on M in the multivariate LKIF framework helps separate the direct information flow $X \rightarrow Y$ from indirect contributions transmitted through M. Meanwhile, a confounder is a variable C that influences both X

and Y ($C \rightarrow X$ and $C \rightarrow Y$); omitting C can bias the estimated coupling by inducing a spurious information flow between X and Y . Z24 demonstrated through theoretical experiments that both the multivariate and bivariate LKIF approaches are valuable for understanding land–atmosphere interactions, even in the presence of mediators and confounders.

While the LKIF has been successfully applied to many problems in geoscience, uncertainties remain regarding the physical limitations of using the bivariate and multivariate forms, especially when applied to land–atmosphere interactions. For instance, Z24 noted that the multivariate and bivariate forms yield similar results in the presence of external variables but did not provide conclusive criteria for when the bivariate LKIF may be compromised or less reliable, and more importantly, the physical limitations leading to their differences. Meanwhile, Docquier et al. (2023) showed that, in a time-invariant LKIF analysis, omitting a key state variable can make 2D and multivariate estimates diverge substantially. Furthermore, interactions in, say, the land–atmosphere continuum, are tightly coupled with overlapping drivers. In such cases, neglecting important variables could lead to inflated or misleading causal strengths and variabilities. Moreover, the influence of these variables is not static but depends on the prevailing land–atmosphere state, where different environmental conditions shape how strongly additional variables contribute to the estimated causal relationships.

This motivates a key question which we explore in this study: under which conditions do the bivariate and multivariate LKIFs differ? More precisely, why would they differ in different locations for the same time period, or differ over time for the same location, even when the same variables are used? This begs a spatio–temporal quality of the role of mediators/confounders in the causal estimation based on LKIF, especially under a nonstationary assumption. In this study, we investigate the importance of conditioners (mediators and/or confounders) in estimating vegetation responses, based on Gross Primary Productivity (GPP) and Leaf Area Index (LAI), to SM and VPD using the Z24 framework. Indications from Z24 suggest that the influence of mediators and/or confounders (both named “conditioners”) may rely on the level of dependency between the cause and the effect variables. Thus, in this study, we leverage this idea to further explore the conditions under which there would be more relevance for mediators and/or confounders in the LKIF estimation. Understanding these dynamics is critical for accurately studying vegetation responses to hydroclimatic drivers.

In the following sections, the datasets and methods are introduced in Sect. 2. Section 3 presents the main results from the real-world application of the LKIF framework. Section 4 discusses the importance of conditioners in shaping causal relationships. Conclusions are presented in Sect. 5.

2 Materials and Methods

2.1 Causality Formalism

The causal inference method applied here is based on the Liang–Kleeman Information Flow (LKIF) causality analysis formalism, which is rigorously derived and formulated from first principles (Liang, 2014, 2016, 2021). In this context, the



causality from one time series (X_2) to another (X_1) is quantified by the rate at which information flows from X_2 to X_1 . Liang (2021) extended this approach to a d -dimensional space to include the influence of potential confounding factors that may impact the relationship between X_2 and X_1 . In a system with d time series, the information flow from X_2 to X_1 , while accounting for mediating/confounding variables, is expressed as (Eq. 1):

$$T_{2 \rightarrow 1|3,4,\dots,d} = \frac{1}{\det C} \cdot \sum_{j=1}^d \Delta_{2j} C_{j,d1} \cdot \frac{C_{12}}{C_{11}} \quad (1)$$

Where $T_{2 \rightarrow 1|3,4,\dots,d}$ is the LKIF from X_2 to X_1 under the influence of various mediators/confounders ($X_3, \dots, X_d$), C is the sample covariance matrix, and $\det C$ is its determinant. Δ_{2j} denotes the cofactor of C . $C_{j,d1}$ represents the sample covariance between X_j and the temporal derivative dX_1/dt using Euler's forward differencing, C_{12} is the sample covariance between X_1 and X_2 and C_{11} is the sample variance of X_1 (for details see Liang, 2021).

Recently, Zhou et al. (2024) extended Liang's multivariate information flow framework by incorporating the Kalman filter to address non-stationarity, resulting in the Multivariate Time-Varying Liang–Kleeman Information Flow (MtvLK) method. This approach allows for the dynamic tracking of causality between multiple time series variables. Within this framework, the Kalman filter estimates the covariance matrix at each time step, which is then used for calculating the time-varying causality between the system's variables. The key equation for MtvLK is (Eq. 2):

$$T_{t2 \rightarrow 1|3,4,\dots,d}(t) = \frac{1}{\det P} \sum_{j=1}^d \Delta_{2j} P_{j,d1} \frac{P_{12}}{P_{11}} \quad (2)$$

Where $T_{t2 \rightarrow 1|3,4,\dots,d}$ is the IF from X_2 to X_1 under the influence of various mediators/confounders ($X_3, \dots, X_d$), where P is the resulting covariance matrix estimated by the Kalman filter and updated at each time step, and $\det P$ denotes its determinant. Δ_{ij} are the cofactors of the matrix P . And $P_{j,d1}$ are the resulting covariance between X_j and the temporal derivative dX_1/dt . P_{12} is the covariance between X_1 and X_2 , and P_{11} is the variance of X_1 (for details, see Zhou et al., 2024).

To evaluate the statistical significance of the Liang–Kleeman information flow at each time step, the information-flow estimate is treated as approximately normally distributed. Its uncertainty is obtained from the maximum-likelihood parameter covariance (inverse Fisher information matrix), and the flow is considered significant when the absolute information flow exceeds the corresponding significance threshold at the chosen level. A controlled synthetic experiment demonstrating the behavior of time-varying LKIF under hidden confounding is provided in Appendix A. The results show that LKIF accurately recovers the correct causal directions and structure even as the strength of unobserved confounding increases. However, differences between bivariate and multivariate IF estimates may arise, reflecting the influence of unobserved confounders/mediators. These findings demonstrate that, while LKIF maintains directional fidelity, conditioning is essential for isolating direct effects and avoiding misinterpretation of causal strength.



In this study, the Information Flow (IF) from SM and VPD to LAI/GPP is quantified, while also accounting for the influence of multiple confounding variables (i.e., SM/VPD, temperature, and surface solar radiation). Within the framework for this study, a coupling is defined as the likelihood of control that one variable has for another, represented by the IF of one variable to another, in the bivariate form, and the likelihood of control in the presence of other variable(s) in the multivariate form. When IF is positive (+IF), this suggests changes in the driver increase the likelihood of extreme (excited) states of the response variable, thus a potential indication of increased vulnerability in the response variable. In contrast, a negative IF (-IF) value indicates that changes in the driver increase the likelihood of an equilibrium (reduced excited states) state of the response variable, and potentially, its increased resilience.

2.2 Differential Information Flow (ΔIF) Calculation

To assess how the causal influence of individual variables (SM or VPD) on vegetation (LAI/GPP) changes in the presence of conditioners (whether mediators or confounders), the differential information flow (ΔIF) is computed. ΔIF is the absolute difference between the bivariate (T^{bi}) and the multivariate (T^{mv}) IF (Eq. 3). Applied to the physical problem here (Eq. 4–5), this metric quantifies the absolute change in IF from SM/VPD to the vegetation (bivariate form) and its multivariate form (taking into account the influences from VPD/SM, T and SSR). Thus, ΔIF of SM and VPD is calculated using the following equations:

$$\Delta_{IF}(t) = |T^{bi}(t) - T^{mv}(t)| \quad (3)$$

$$\Delta_{SM}(t) = |T^{SM \rightarrow LAI \setminus GPP}(t) - T^{SM \rightarrow LAI \setminus GPP | VPD, T, SSR}(t)| \quad (4)$$

$$\Delta_{VPD}(t) = |T^{VPD \rightarrow LAI \setminus GPP}(t) - T^{VPD \rightarrow LAI \setminus GPP | SM, T, SSR}(t)| \quad (5)$$

Based on the computed ΔIF values, we assess the conditions under which the multivariate IF diverges (converges) from (to) the bivariate form. A small ΔIF indicates that the bivariate form is very similar to the multivariate one. In such cases, the inclusion of additional variables does not notably alter the causal influence, implying that the key causal pathway is already captured in the bivariate relationship with little dependency on mediators and/or confounders. Conversely, a large ΔIF suggests that the causal influence is substantially modified when additional variables are introduced, indicating a more complex causal relationship. In this case, mediators and/or confounders provide additional significant information that reshapes the apparent causal structure. It is essential to note that the change in causal structure by incorporating other variables does not necessarily imply that the bivariate form is incorrect in isolating dependencies, but rather that the quantitative information gathered is not accurate. As discussed in Vannitsem et al. (2024), in a simplified setting, the addition of observables can indeed modify the amplitude or sign of the influence but not the importance of the considered variable in the causal relationship uncovered. The emergence of spurious LKIF is, however, possible as illustrated in Docquier et al. (2023).



To assess the statistical significance of the ΔIF between paired conditions (e.g., with vs. without a mediator), a paired two-tailed Student's t-test was applied at each time step. A 95% Confidence Interval (CI) for the difference in means was computed, and ΔIF was considered statistically significant when the CI did not include zero (equivalent to $p < 0.05$).

160 2.3 Information-based correlations (rIF)

In some cases, large differences may exist between the multivariate and bivariate forms; however, the correlations between their time-varying estimates could be very high, implying that they capture the same physical process but at different magnitudes. Therefore, we also assess the Pearson correlation (rIF) between the time-varying bivariate information flow and the time-varying multivariate one. This allows us to obtain a more holistic view of the conditions for divergence between the bivariate and multivariate IFs. For regime-specific behavior, rIF is restricted to the subset of months belonging to a defined regime (Eq. 6):

$$rIF = |corr(T_{bi}(t), T_{mv}(t))_{\text{regime}}| \quad (6)$$

In this study, we use the absolute correlation ($|rIF|$), focusing on the strength of the temporal covariation. Here, we bin the time series of SM and VPD into four quantile-based regimes, yielding a 4x4 grid of combined regimes, corresponding to the combinations of SM and VPD quartiles (Q1, Q2, Q3, Q4 for each). The SM quartiles range from Q1, representing the driest conditions, to SM at Q4, representing the wettest conditions. Meanwhile, VPD quartiles range from Q1 (lowest demand) to Q4 (highest demand). For each quartile, we calculate rIF and the median of ΔIF .

2.4 Mediator-Based Decomposition of Information Flow Divergence

Understanding why T^{mv} diverges from T^{bi} leads us to derivable measures to quantify the relevance of the mediators/confounders. To determine how individual mediators, modify the inferred causal influence between each driver-target pair, the differential Information Flow signal $\Delta IF(t)$ was decomposed into contributions (Eq. 7–9) from progressively expanded conditioning sets. Let $T^{bi}(t)$ denote the bivariate IF from the driver (SM or VPD) to the target variable (LAI or GPP) and let $T^{mv|m}(t)$ denote the corresponding multivariate IF conditioned on a conditioner set (m_1, m_2, m_3). For a coupling and a sequence of conditioners, the decomposition follows,

$$180 \quad \Delta IF_{m_1}(t) = T^{bi}(t) - T^{bi} | m_1(t) \quad (7)$$

$$\Delta IF_{m_2}(t) = T^{bi} | m_1(t) - T^{bi} | m_1, m_2(t) \quad (8)$$

$$\Delta IF_{m_3}(t) = T^{bi} | m_1, m_2(t) - T^{bi} | m_1, m_2, m_3(t) \quad (9)$$



This decomposition allows us to examine which mediator contributes most to the divergence, and in what direction (suppression or enhancement). From here, we summarize how each conditioner contributes to the restructuring of Information Flow based on four indices (Eq. 10–13) computed from the temporal components $\Delta IF_m(t)$.

2.4.1 Mediator Dominance Index (MDI)

The Mediator Dominance Index (MDI) quantifies the proportion of the conditioner (m) that contributes the most to the total magnitude of information-flow restructuring (Eq. 10):

$$MDI_m = \frac{\sum_t |\Delta IF_m(t)|}{\sum_m \sum_t |\Delta IF_m(t)|} \quad (10)$$

Large MDI_m values identify conditioners that dominate the divergence between bivariate and multivariate couplings.

2.4.2 Moderation Gain (MG)

Moderation Gain (MG) shows how strongly the conditioner (m) increases the inferred coupling. The gain is defined as (Eq. 11);

$$MG_m = \sum_t \max(0, \Delta IF_m(t)), \quad (11)$$

High MG_m values identify conditioners that dampen the apparent driver influence in the bivariate signal.

2.4.3 Confounding Pressure (CP)

Confounding Pressure (CP) measures how strongly the conditioner (m) suppresses inflated bivariate influence and is given in Eq. 12;

$$CP_m = \sum_t \max(0, -\Delta IF_m(t)) \quad (12)$$

Large CP_m values indicate strong confounding by the conditioner.

2.4.4 Convergence Rate (CR)

Convergence Rate (CR) quantifies how often the bivariate estimate is close to the fully conditioned estimate. We define the CR using the absolute divergence threshold ε_{abs} (Eq. 13);

$$CR = \frac{1}{N} \sum_t (|\Delta IF(t)| \leq \varepsilon_{abs}) \quad (13)$$



205 Here ε_{abs} is chosen as a fixed tolerance reflecting a physically meaningful scale of information-flow variation (e.g. the 10th percentile of ΔIF across all couplings). High CR values indicate that the bivariate coupling is sufficiently close to the multivariate form during a large fraction of the analyzed period.

2.5 Data

210 The Gross Primary Productivity (GPP) data, reflecting photosynthetic activity of plants, and Leaf Area Index (LAI, representing vegetation greenness, utilized in this study, are obtained from the Global Land Surface Satellite (GLASS) dataset (Liang et al., 2021). The data has a spatial resolution of 0.05° and a temporal resolution of 8 days, covering the period from 1982 to 2018. For consistency with other variables in the analysis, the dataset is resampled to a spatial resolution of $0.25^\circ \times 0.25^\circ$ (longitude $\times$ latitude), using bilinear interpolation and then aggregated to monthly timescales. Due to reported uncertainties in data quality before 2002, the present study utilizes data spanning from 2004 to 2018.

215 The monthly data on Volumetric Soil Moisture (SM), 2-m air temperature, and Surface Solar Radiation (SSR) used in this study are obtained from European Centre for Medium-Range Weather Forecasts' (ECMWF) datasets, with SM taken from ERA5-Land and temperature and SSR from ERA5 global atmospheric reanalysis products, covering the period from 2004 to 2018. The weighted average of SM, computed between 0 and 289 cm (all four layers of SM), is used here, with the weights corresponding to the thickness of each layer (0–7, 7–28, 28–100, and 100–289 cm). The original resolution of the SM data
 220 ($0.1^\circ \times 0.1^\circ$) is subsequently re-gridded at a horizontal resolution of $0.25^\circ \times 0.25^\circ$. Vapor pressure deficit (VPD) is estimated using ERA5's 2-m minimum and maximum temperature and 2-m dewpoint temperature (Upreti & Ojha, 2017). The monthly anomalies for all variables are computed for the period from January 2004 to December 2018 by subtracting the respective climatological means from the original data.

3 Results

225 3.1 Real-world applications in land–atmosphere interactions

Figure 1 illustrates the coupling strength from SM/VPD to LAI (a-b) and from SM/VPD to GPP (c-d), estimated via Information Flow (IF), for two humid forest biomes: Southeast China ($114.25\text{--}117.25^\circ\text{E}$, $25.25\text{--}28.25^\circ\text{N}$) and the Amazon Basin ($54\text{--}60^\circ\text{W}$, $10\text{--}15^\circ\text{S}$), over the period from 2004 to 2018. The locations of these study regions are shown in Supplementary Fig. S1. Across both regions, the LKIF analysis captures the temporal evolution of vegetation response to
 230 hydroclimatic variability and reveals when conditioning on mediating variables (VPD, T, SSR) alters or preserves the direct causal pathways.

a. Role of Conditioners in the Couplings between Soil Moisture / Vapor Pressure Deficit and Vegetation



In the Southeast China region (Fig. 1a, top panel), the SM→LAI coupling is weak and mostly insignificant during 2004–2008. From 2008 onward, the coupling strengthened noticeably, peaking in 2011 with significant positive IF, demonstrating the increasing importance of SM for the structural variability of vegetation during this period. Conditioning on other variables (SM→LAI | VPD; SM→LAI | VPD, T; SM→LAI | VPD, SSR; SM→LAI | VPD, T, SSR) produces only minor changes in magnitude, showing that the bivariate signal is not strongly confounded by the atmospheric factors used here because the SM influence dominates. The overall positive IF suggests that changes in SM increase the likelihood of vegetation structural vulnerability in the region.

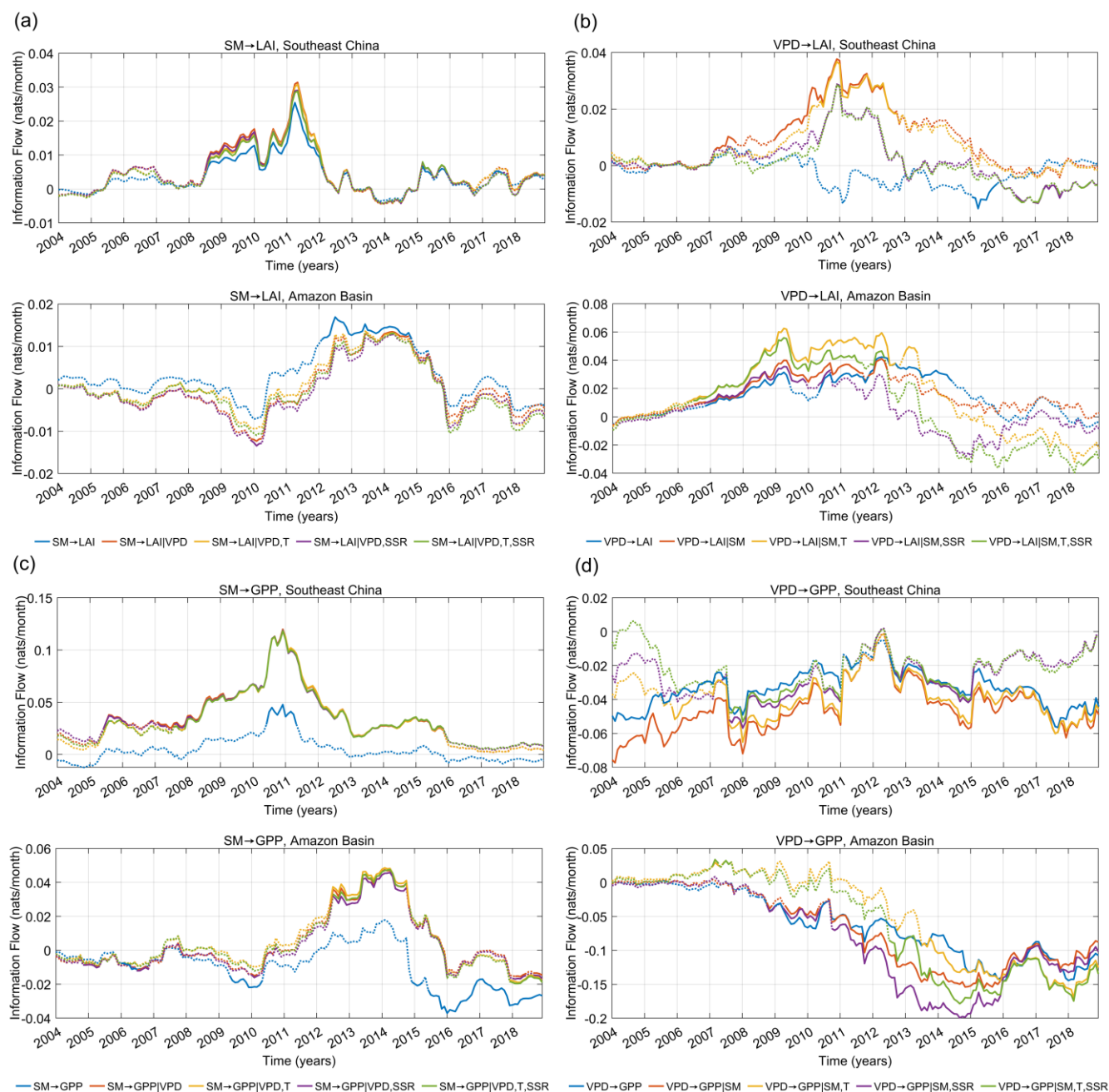
In the Amazon Basin (Fig. 1a, bottom panel), the SM→LAI pathway shows broadly similar temporal variability in both the bivariate and multivariate estimates, indicating a generally strong hydrological influence on canopy structure. However, the bivariate estimate remains larger than the multivariate estimates throughout the whole period (except in 2014–2015, when values are very similar), indicating the confounding/mediating influence of other drivers. From 2004 to 2009, IF gradually declined toward negative values with a small fluctuation in 2007, suggesting increased structural resilience due to SM, though IF remains statistically insignificant throughout this period. Between 2010 and 2014, IF increased sharply, indicating heightened vegetation structural vulnerability to moisture variability. The bivariate IF becomes significant after 2012, reflecting an apparent strengthening of the SM→LAI relationship. However, after conditioning on mediating/confounding variables (SM→LAI | VPD; SM→LAI | VPD, T; SM→LAI | VPD, SSR; SM→LAI | VPD, T, SSR), this significance disappears. The loss of significance indicates an apparent more direct SM→LAI. In the years after 2014, the IF decreases, suggesting reduced vegetation vulnerability. Accounting for the conditioners results in only minor adjustments to IF magnitude, showing that removing atmospheric influences does not substantially alter the direct SM→LAI coupling. Overall, although atmospheric variables exert secondary effects, soil moisture remains the primary driver of canopy structural variability.

Figure 1b shows the VPD→LAI IFs in the two regions. The top and bottom panels show rather different temporal behaviors in the bivariate and multivariate IFs compared to Fig 1a. In this case, introducing confounding/mediating variables (VPD→LAI | SM; VPD→LAI | SM, T; VPD→LAI | SM, SSR; VPD→LAI | SM, T, SSR) substantially modifies the coupling behavior. However, this behavior remains time-dependent, after 2007, conditioning on the other variables leads to a stronger modification, with the divergence between the bivariate and multivariate forms increasing in both regions. In Southeast China, we even find different IF signs between the bivariate and multivariate forms from 2010 to 2016. From 2016 onwards, both regions show greater variability in IF signs across the multivariate forms. These suggest more complex VPD_driver-based couplings for vegetation structure than SM_driver-based couplings.

Figures 1c–d show IFs of SM/VPD to GPP, and their multivariate forms for both regions. As was found in Fig. 1a–b, the GPP effect-based couplings also show in both regions that conditioning on the other variables results in little adjustments and similar trends in the SM driver-based couplings, while more variations are seen in the VPD driver-based couplings. The changes



265 towards positive or negative IF are strongly impacted by ecosystem stress, here more consistent with drought occurrences in the region (Sun and Yang, 2012; Feldpausch et al., 2016). These results reveal that dependency on conditioners is both spatially and temporally sensitive, given the same variables. Thus, the practice of just conditioning on other variables, under a stationary assumption, should be done with caution.





270 **Figure 1: Time series of the information flow (IF) for Southeast China and the Amazon basin (2004 to 2018) for both bivariate and multivariate forms. (a) From SM to LAI, (b) From VPD to LAI, (c) From SM to GPP, (d) From VPD to GPP. Dotted lines represent the overall LKIF, while solid lines indicate statistically significant IF. (LAI= Leaf Area Index, GPP= Gross Primary Production, SM= Soil Moisture, VPD= Vapor Pressure Deficit, T= Temperature, SSR= Surface Solar Radiation).**

3.2 When are Conditioners Important? Δ -Information-Flow Analysis

275 To further explore the conditions under which more divergence/convergence (large/small Δ IF) between bivariate and multivariate estimates occur in the application above, we further analyze the temporal evolution of Δ IF for both SM/VPD $\rightarrow$ LAI and the SM/VPD $\rightarrow$ GPP pathways across Southeast China and the Amazon Basin. Δ IF indicates the degree of convergence/divergence between the bivariate and multivariate IFs. Here, for the multivariate form, we include all confounding variables used in this study. Figure 2(a,d) shows the Δ IF of SM/VPD $\rightarrow$ LAI (Δ SM: blue plots, Δ VPD: red plots),
 280 and Fig. 2(g,j) shows the same as Fig. 2(a,d) but for GPP. Figure 2(a,d) consistently shows high convergence in Δ SM in both regions across all times, while Δ VPD shows more time-dependent divergence. The ability of the Z24 to capture immediate changes in IF plays a pivotal role in shaping these differences. These results indicate that the SM $\rightarrow$ LAI coupling is direct, as Δ SM is very small, with negligible influence from mediators/confounders, reflecting a strong hydrological control on canopy structure in these biomes. In contrast, Δ VPD exhibits marked fluctuations and alternates between positive and negative phases.
 285 Generally, atmospheric water demand (VPD) would depend on land water supply (SM), clear skies (increased SSR), and how these increases or decrease T, to impact vegetation density (Ficklin & Novick, 2017; Yuan et al., 2019; Zhou et al., 2019). Furthermore, VPD is very sensitive to changes in these conditioners, especially the atmospheric ones, making it more responsive to their impacts. This sensitivity suggests why conditioning on these variables changes the apparent strength of VPD's impact on vegetation.

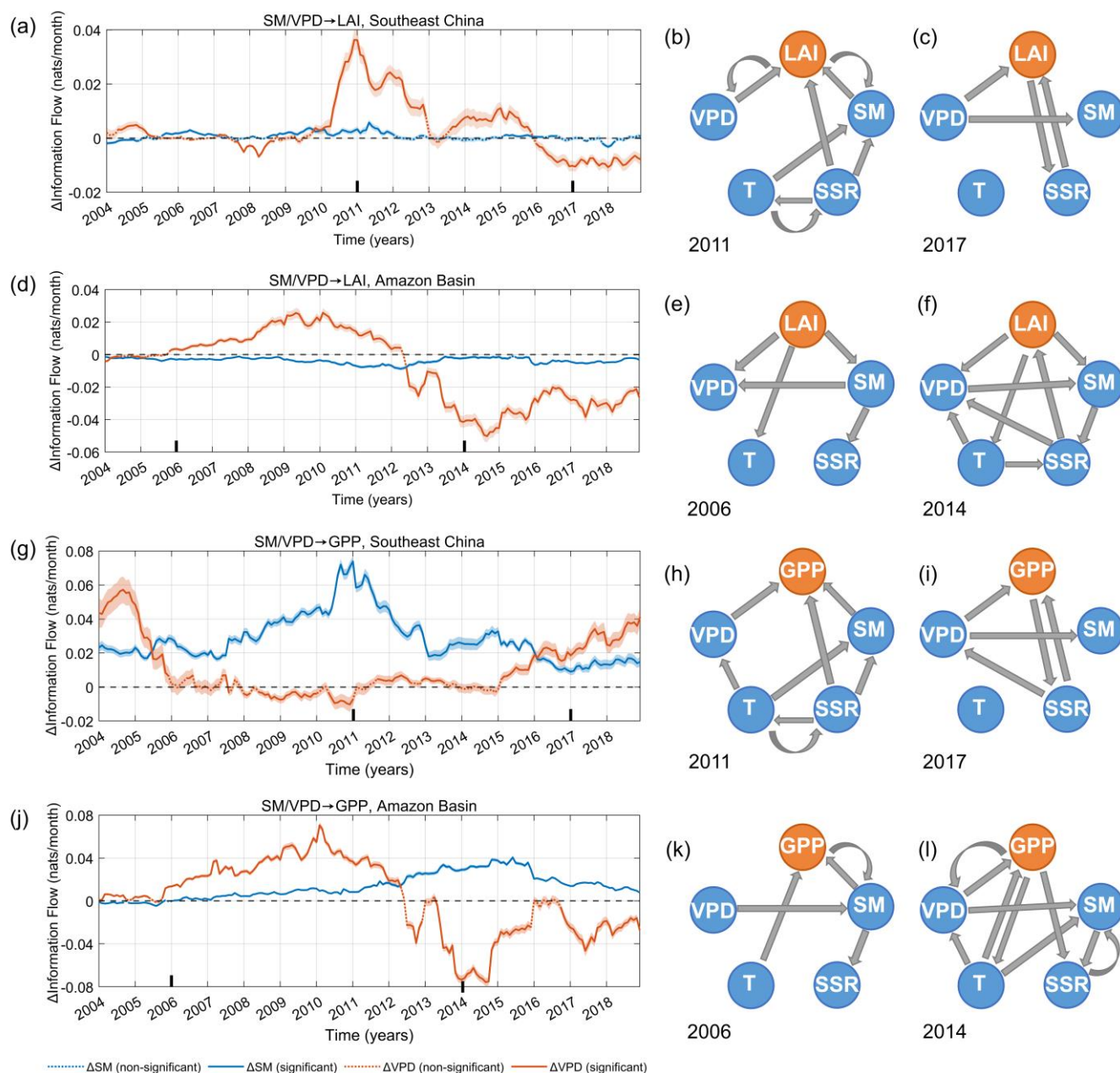
290 The GPP effect-based Δ IF shows largely different patterns compared to the LAI effect-based Δ IF. Firstly, while Fig. 2(a,d) shows consistently convergent patterns across the whole time period for Δ SM in both regions, we find time-varying changes in Δ SM in Fig. 2(g,j), although this is more distinct in Southeast China than in the Amazon Basin. This implies that while SM has a more direct impact on LAI, it is a less direct driver of GPP. On the other hand, Δ VPD shows rather different patterns across both regions. In southeast China, Δ VPD shows continuously high convergence during most of the time period; however,
 295 as with Δ SM, it is characterized by fluctuations and alternates between positive and negative phases. Thus, VPD $\rightarrow$ GPP coupling is more direct in Southeast China than in the Amazon Basin.

Figure 2(a,d,g,j) shows that regions with rich/strong coupling/feedback, particularly the Amazon Basin, exhibit large differences in Δ IF, indicating substantial divergence between the bivariate and multivariate pathways.

To dig deeper into the potential reasons for these nuanced patterns of Δ IF, we illustrate the causal graphs for (1) a time-point
 300 where Δ IF is large (stronger divergence) and (2) a time point where Δ IF is small (stronger convergence) for both regions (Fig.



2b–c, e–f, h–i, k–l). The results suggest that stronger divergence is associated with richer coupling/feedback time points, while stronger convergence occurs when there are fewer couplings. These results agree with a previous study, which suggested that couplings/feedback reduce under drought conditions (Ruddell & Kumar, 2009). This could also explain why ΔVPD converges in Southeast China around the neighborhood time of 2011, since these periods were marked by recurrent droughts in the region (Sun and Yang, 2012). Under such drier conditions, VPD becomes a more dominant driver of vegetation, consistent with the findings of a recent study (Yuan et al., 2019). These results illustrate how ΔIF variability translates into shifts in the underlying causal structure. High- ΔIF years correspond to more complex, mediator-driven pathway configurations, whereas low- ΔIF years reflect simpler and predominantly direct interactions.



310 **Figure 2: Time series of differential Information Flow (ΔIF) for Southeast China and the Amazon Basin (2004–2018). (a,d) for**
SM/VPD to LAI, and (g,i) from SM/VPD to GPP. Solid lines denote periods where ΔIF is statistically significant ($p < 0.05$); dotted
lines indicate non-significant values. Shaded bands represent the 95% confidence interval. ($\Delta SM = |TSM \rightarrow LAI/GPP - TSM \rightarrow LAI/GPP|VPD, T, SSR|$ and $\Delta VPD = |TVPD \rightarrow LAI/GPP - TVPD \rightarrow LAI/GPP|SM, T, SSR|$). Vertical tick marks denote the time
points selected for causal graph construction. Summary of the causal graphs for years exhibiting large and small IF divergence for
 315 **LAI (b–c, e–f), and for GPP (h–i, k–l). Stronger ΔIF corresponds to years with richer coupling and feedback structure, whereas**



smaller ΔIF reflects periods with fewer couplings. (LAI= Leaf Area Index, GPP= Gross Primary Production, SM= Soil Moisture, VPD= Vapor Pressure Deficit, T= Temperature, SSR= Surface Solar Radiation).

3.3 State-Dependent patterns of changes in information flow

To further assess when and where bivariate and multivariate IFs estimates diverge, we computed the differential information flow ($|\Delta IF|$, Section 2.2) and the information-based correlation ($|rIF|$, Section 2.3). To jointly visualize the two diagnostics across the combined regimes, we use the split-triangle heatmap layout. For each 4×4 panel, we overlay grid lines, label the axes by SM and VPD quartiles, and hatch any cells with zero samples using diagonal stripes; this immediately flags regimes where no robust causal inference is possible. This is routinely repeated for all four couplings, focusing on southern China, to show how $|\Delta IF|$ and $|rIF|$ between bivariate and multivariate IF depend jointly on SM and VPD regimes.

The SM→LAI pathway (Fig. 3a), exhibits uniformly high rIF and low ΔIF across nearly all SM–VPD quartile combinations. This concentrated pattern demonstrates that the SM–LAI coupling is both strong and consistently direct, with minimal differences between bivariate and multivariate IF estimates. The uniformity across hydroclimatic states indicates that vegetation structural responses to soil moisture in humid forests are stable and largely insensitive to atmospheric variables. In contrast, the SM→GPP (Fig. 3c) shows high correlation and larger ΔIF values. Although the SM–GPP coupling remains strong across quartiles (as revealed by the large correlation), the pronounced difference in information flow between the bivariate and multivariate forms indicates that mediator inclusion alters the estimated causal strength more substantially than in the SM→LAI case. This reflects the higher complexity of productivity (GPP) responses relative to canopy structure (LAI); GPP integrates more processes and is therefore more sensitive to the removal of atmospheric confounding.

The VPD→LAI and VPD→GPP pathways (Fig. b-d) show wider variability in both rIF and ΔIF . Correlations range from weak to strong, and ΔIF spans small to large magnitudes across quartiles. This broad spread highlights the more nonlinear and state-dependent behavior of VPD-driven couplings. Supplementary Fig. S2(a-c) shows the detailed ΔIF structure across regimes of water supply and atmospheric demand for all conditioning levels.

Overall, Fig. 3 shows that SM-based couplings (a-c) exhibit much greater uniformity than VPD-based couplings (b-d). The SM panels display consistent correlation strength and ΔIF patterns, whereas the VPD panels show substantial variation in both metrics. This suggests that VPD-driven interactions are more sensitive to environmental conditions and may require additional conditioning variables to achieve the stability seen in SM-driven couplings.

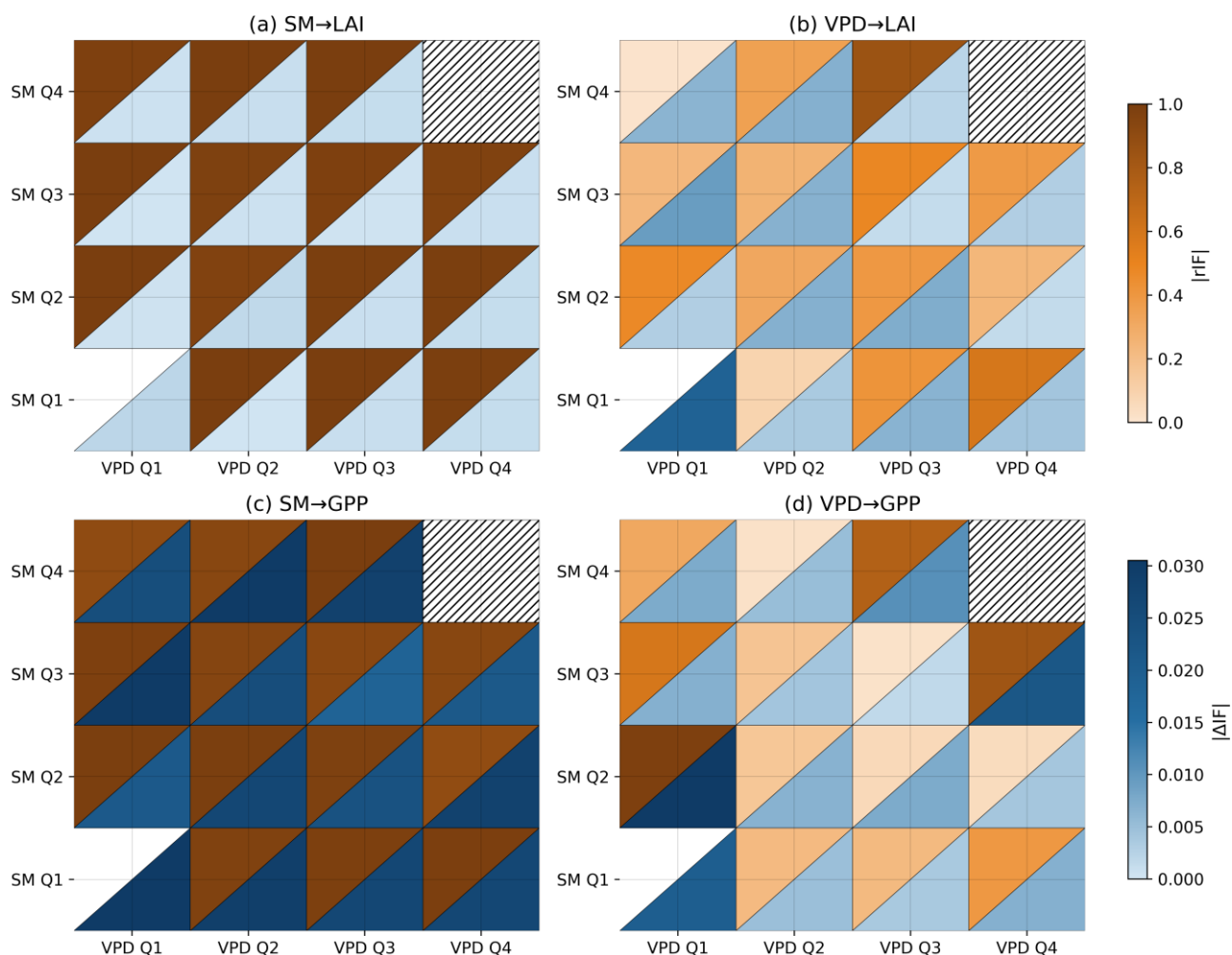


Figure 3: Differences (ΔIF) and correlations (rIF) between bivariate and multivariate Information Flow across SM and VPD quartiles (Q1–Q4) for Southeast China. (a) SM→LAI, (b) VPD→LAI, (c) SM→GPP, and (d) VPD→GPP. Each cell is divided into an upper triangle ($|rIF|$: magnitude of Pearson correlation 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. Cross-hatched cells indicate quartile combinations with no data. (SM= Soil Moisture, VPD= Vapor Pressure Deficit, LAI= Leaf Area Index, GPP= Gross Primary Production).

3.4 ANOVA of Regime-dependent Changes in Information Flow



350 This ANOVA framework (Appendix B) provides a formal variance-partitioning approach to identify the hydroclimatic conditions under which mediator removal alters coupling strength most strongly, thereby isolating the environmental regimes that drive the largest departures between bivariate and fully conditioned information-flow estimates.

a. Two-way ANOVA: moisture–demand control of $|\Delta IF|$

355 Across all four pathways (SM→LAI, VPD→LAI, SM→GPP, VPD→GPP), the SM and VPD regimes exert a clear influence on the magnitude of $|\Delta IF|$ (Fig. 4a). For the SM-driven pathways, the SM main effect dominates, indicating that differences between bivariate and multivariate estimates grow primarily across the wet–dry gradient. VPD contributes very little to $|\Delta IF|$ for these pathways, reinforcing that LAI and GPP responses to SM are largely direct and only weakly mediated by atmospheric demand.

360 For VPD-driven pathways, the SM×VPD interaction is the only meaningful component, showing that the divergence between bivariate and multivariate pathways is controlled mainly by the combined moisture–demand regime rather than by either factor independently. These patterns reveal that LAI pathways exhibit small $|\Delta IF|$ and weaker regime sensitivity, whereas GPP pathways show larger $|\Delta IF|$ and stronger dependence on moisture–demand structure. The largest departures occur under compound dry and high-VPD conditions.

b. Thermal modulation: SM×VPD×T structure

365 Introducing temperature as a third factor (Fig. 4b) substantially increases the explanatory power of the ANOVA for the GPP pathways. The T main effect is pronounced for both SM→GPP and VPD→GPP, indicating that hot regimes amplify differences between bivariate and multivariate causal estimates. This reflects the strong co-variation between T and VPD during warm months, which intensifies atmospheric demand and modifies the relative contributions of SM and VPD to ecosystem functioning. High-order interactions involving T, notably VPD×T and SM×VPD×T, explain large fractions of
 370 variance in $|\Delta IF|$ for GPP. These terms demonstrate that differences between bivariate and fully conditioned estimates arise not only from moisture or demand individually but from their joint modulation under thermal stress. For the LAI pathways, temperature effects remain detectable but generally weaker, consistent with the slower structural response of canopy development.

c. Radiative modulation: SM×VPD×SSR structure

375 Surface solar radiation further modulates the divergence between bivariate and multivariate couplings (Fig. 4c). The SSR main effect is most evident for the GPP pathways, indicating that bright conditions heighten the influence of moisture and demand on the inferred causal structure. Under high radiation, photosynthesis becomes increasingly limited by stomatal regulation and water supply, making SM–VPD–SSR interactions more dominant.

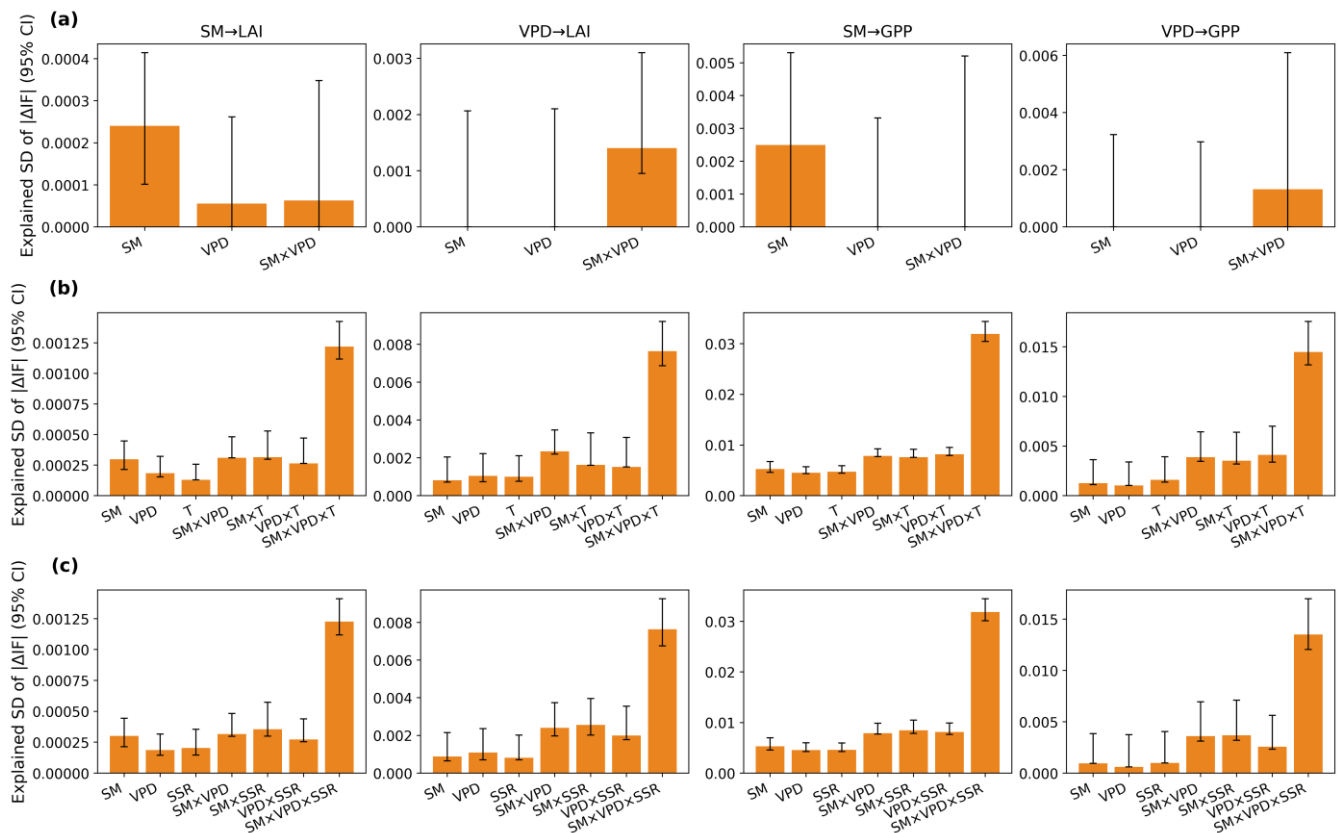


Figure 4: ANOVA results showing the explained standard deviation ($\sqrt{\text{AEV}}$) of $|\Delta\text{IF}|$ for Southeast China. Columns represent the four pathways: SM→LAI, VPD→LAI, SM→GPP, and VPD→GPP. (a) Two-way ANOVA with factors SM and VPD. (b) Three-way ANOVA including SM, VPD, and T. (c) Three-way 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= Solar Surface Radiation). Note that the Y-axis range differs in each panel to better see the different values.

The SM×SSR and VPD×SSR interactions explain sizable fractions of the variance for SM→GPP and VPD→GPP, respectively, demonstrating that the largest changes in ΔIF arise under bright–dry and bright–high-demand conditions. The three-way SM×VPD×SSR interaction is also non-negligible, particularly for the GPP pathways, indicating that the breakdown of bivariate couplings is strongest under simultaneously dry, high-VPD, and high-radiation regimes. Whereas, LAI pathways exhibit weaker radiative interactions, reflecting their slower structural adjustment timescale and lower instantaneous sensitivity to radiative conditions. The corresponding variance fractions (ω^2) for each pathway are shown in Supplementary Fig. S3.

Altogether, the ANOVA results show that the divergence between bivariate and multivariate couplings is strongly regime dependent and reaches its maximum under compound environmental stress. The largest explained standard deviation (SD) values occur in dry–high-VPD regimes, particularly when combined with hot or high-radiation conditions, indicating that the



system's causal architecture fundamentally changes under simultaneous supply, demand, and energy limitations. In these states, strong SM×VPD and SM×VPD×energy (T or SSR) interaction terms reveal that multiple constraints act jointly on the ecosystem, causing the bivariate IF to conflate several distinct processes. Importantly, the analysis also reveals a clear difference between structural and functional responses: LAI-based couplings exhibit minimal regime dependence and consistently small explained SD, reflecting their stable and weakly mediated behavior. In contrast, GPP-based couplings show much larger explained SD and strong sensitivity to moisture–demand–energy interactions, demonstrating that GPP responds nonlinearly to compound stress and is far more strongly mediated than LAI.

4. Discussion: Diagnosing the importance of conditioners

Based on the results so far, we provide four indices that could be used to summarize how individual mediators/confounders reshape the couplings by examining: (1) mediator dominance (MDI), (2) moderation gain (MG), (3) confounding pressure (CP), and (4) convergence rate (CR). Here, we select the SM_cause-based couplings in Southeast China to simplify the demonstration. We thus highlight why SM→LAI and SM→GPP couplings behave so differently in terms of ΔIF . We note that for the purposes of this study, all the definitions provided here are strictly with respect to the Liang-Kleeman information flow.

MDI (Fig. 5a) quantifies the relative share of $|\Delta IF|$ attributable to each mediator. VPD emerges as the dominant mediator for both pathways, but especially for SM→GPP. For SM→LAI, VPD accounts for roughly two-thirds of the total $|\Delta IF|$, while the remainder is distributed between T and SSR. This indicates that although VPD is the primary contributor, ΔIF for SM→LAI still reflects multiple environmental influences. In contrast, the SM→GPP pathway is almost entirely driven by VPD-related restructuring, with MDI close to 1 and only minor contributions from temperature and radiation. This concentration reveals that the discrepancy between bivariate and multivariate SM→GPP couplings is predominantly determined by VPD co-variation.

MG (Fig. 5b) captures the sum of positive ΔIF values and identifies mediators that amplify the deviation between bivariate and multivariate IF. For SM→LAI, MG is small for all mediators, increasing slightly from VPD to T and reaching its largest values for SSR. This pattern shows that radiative and thermal conditions modestly enhance departures from the bivariate estimate, whereas VPD contributes relatively little positive deviation. In stark contrast, SM→GPP exhibits strong MG dominated by temperature: T produces far larger moderation gain than VPD or SSR. Warm conditions, therefore, play a central role in amplifying GPP-related ΔIF , with SSR providing additional but smaller contributions.

CP (Fig. 5c) measures the accumulated negative ΔIF and therefore the degree to which mediators inflate the bivariate coupling relative to the multivariate one. SM→LAI displays very low CP, indicating minimal inflation of its bivariate estimate and confirming that its bivariate IF is only weakly distorted by confounding. SM→GPP, however, shows large CP, revealing that



confounding from VPD, T, and SSR substantially exaggerates the apparent SM→GPP influence. This confirms that the bivariate representation of SM→GPP can markedly overstate the true conditioned coupling.

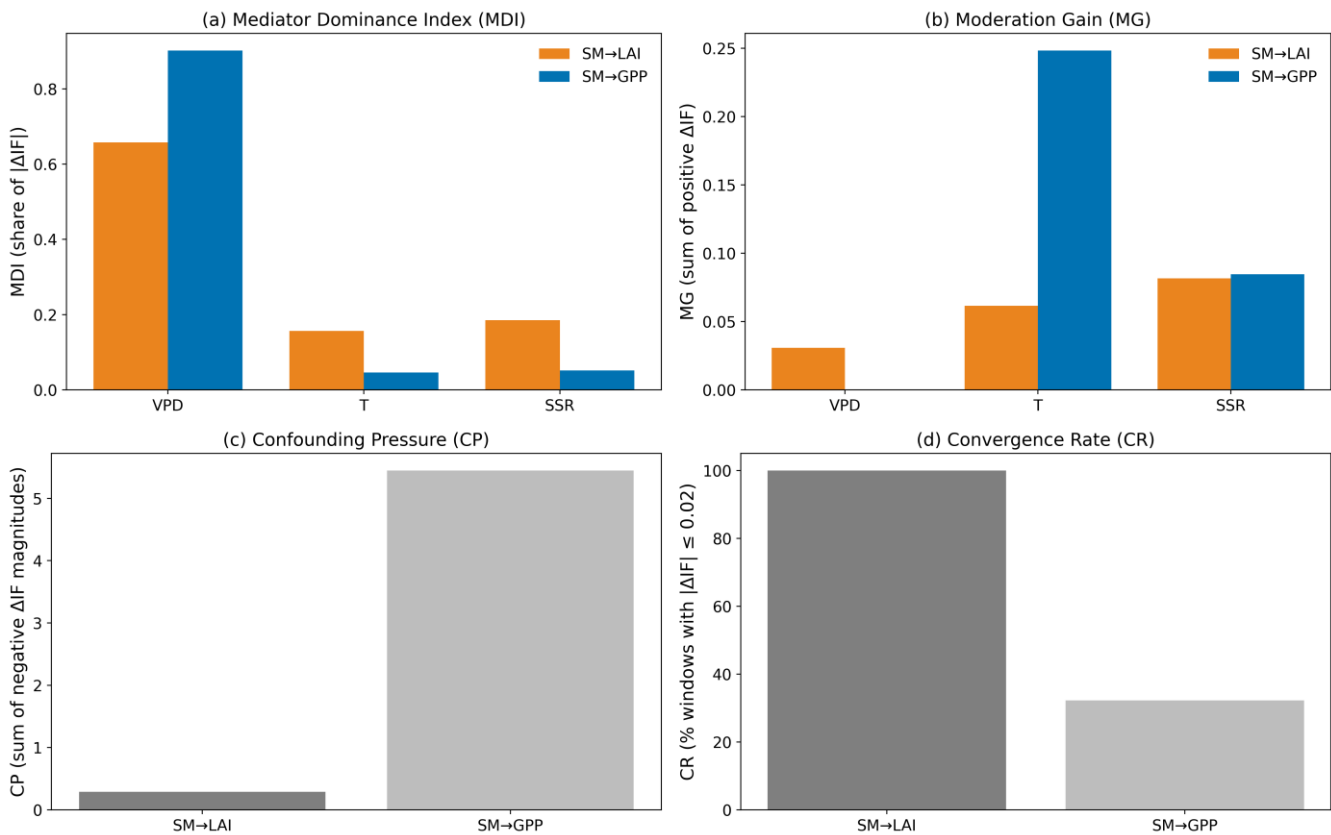


Figure 5. Importance of conditioning variables for $|\Delta IF|$ based on (a) Mediator Dominance Index (MDI), (b) Moderation Gain (MG), (c) Confounding Pressure (CP), and (d) Convergence Rate (CR), for the SM→LAI and SM→GPP couplings in Southeast China.

CR (Fig. 5d) quantifies the percentage of time windows in which $|\Delta IF|$ remains below a small threshold and thus reflects how often the bivariate estimate is effectively sufficient. SM→LAI has a CR near 100%, indicating that the bivariate and multivariate IF almost always agree and that conditioning on mediators is rarely necessary. In contrast, SM→GPP shows a much lower CR, meaning that the bivariate estimate frequently diverges from the multivariate one, and mediator conditioning is essential for an accurate causal representation.

Figure 5 demonstrates a clear structural–functional divide in vegetation–climate coupling. The SM→LAI pathway is structurally simple and largely causally sufficient: mediator effects are small, confounding pressure is negligible, and bivariate and multivariate IF show consistent agreement. In contrast, the SM→GPP pathway is strongly mediator-dependent. VPD dominates its ΔIF structure, temperature and radiation amplify deviations, and confounding pressure materially affects its



bivariate representation. These findings show that some vegetation couplings (e.g., $SM \rightarrow LAI$) are robust and require minimal conditioning, whereas other pathways, such as $SM \rightarrow GPP$, depend critically on accounting for mediator effects to correctly characterize their causal behavior. The corresponding SM – VPD quartile-specific results are shown in Supplementary Fig. S4.

440 5. Conclusion

This study investigated when and why conditioners may alter information flow pathways. We achieve this by analyzing divergence between the bivariate and multivariate formulations of Liang–Kleeman Information Flow, and how these differences reflect the contribution of the conditioners to an application in land–atmosphere interactions. A synthetic validation (Appendix A) showed that LKIF preserves directional fidelity under hidden confounding, though differences between bivariate
 445 and multivariate estimates still occur.

A real-world application revealed that the impacts of conditioners on causal structures vary across time and space, demonstrating that spatial and temporal averaging could mask the relevance of conditioners. In our study, $SM \rightarrow LAI$, representing vegetation structure, showed consistently more direct behavior in different locations across different periods of time, with minimal mediator influence, and high causal sufficiency. In contrast, $SM \rightarrow GPP$, representing vegetation function,
 450 exhibited strong mediator dependence, substantial divergence, and marked temporal variability. These differences were particularly pronounced during periods of compound stress, when atmospheric demand, temperature, or radiation jointly altered the inferred causal pathway. VPD emerged as the dominant mediator shaping ΔIF for $SM \rightarrow GPP$, while temperature showed the largest increase in the coupling when included as a conditioner. Together, these patterns demonstrate that conditioning variables are essential for functional pathways but comparatively unimportant for structural ones.

We also found that the physical states of the driver variables further controlled the degree of divergence. SM -driven couplings showed stable behavior across supply–demand states, whereas VPD -driven pathways displayed wide variability in both rIF and ΔIF . ANOVA confirmed that the largest departures occurred under combinations of dryness, high VPD , and elevated T/SSR conditions known to intensify plant stress. These state-dependent effects explain why mediators appear intermittently, because their influence strengthens only when climatic conditions amplify dependencies among drivers. Importantly, this study
 460 shows that when driver-response relationships are predominantly more direct, mediators/confounders contribute little (Docquier et al., 2024). However, under more complex or compound-stress conditions, mediators/confounders become critical to capture the underlying causal mechanisms.

While this work does not include all potential mediators, the selected variables represent dominant environmental controls and yield physically interpretable causal signals. The IF framework provides a transparent, first-principles basis for causal
 465 estimation; however, future work should explore nonlinear extensions (Pires et al., 2024; Vannitsem et al., 2025) to better capture complex feedbacks that arise during extreme events.



Our findings provide conceptual and practical frameworks for deciding when conditioning is necessary and highlight the importance of considering mediators in future applications of Information Flow to land–atmosphere systems. Furthermore, there is a potentially important application for feature selection for machine learning model development, which is yet to be explored.

Appendix A: Theoretical experiments

We begin by demonstrating how hidden confounders influence information-flow estimation through a controlled synthetic experiment. The goal is to assess whether LKIF can still recover a faithful causal structure when parts of the underlying system are unobserved, a situation frequently encountered in Earth-system applications. The experiment uses a five-dimensional, linear, stable Vector Autoregressive (VAR1) process defined as (Eq. A1);

$$\mathbf{x}_t = A\mathbf{x}_{t-1} + \boldsymbol{\varepsilon}_t, \quad \boldsymbol{\varepsilon}_t \sim \mathcal{N}(0, \Sigma), \quad (\text{A1})$$

Where $\mathbf{x}_t = (x_{1,t}, x_{2,t}, x_{3,t}, x_{4,t}, x_{5,t})^\top$ are the five different time series and $\Sigma = \text{diag}(b_1^2, b_2^2, b_3^2, b_4^2, b_5^2)$, with b_i being the stochastic perturbation amplitudes. The coefficient matrix A is (Eq. A2);

$$A = \begin{pmatrix} \phi & c_{21} & c_{31} & \gamma & 0 \\ c_{12} & \phi & c_{32} & \gamma & 0 \\ 0 & 0 & \phi & 0 & 0 \\ 0 & 0 & 0 & \phi & \eta \\ 0 & 0 & 0 & 0 & \phi \end{pmatrix} \quad (\text{A2})$$

encodes all causal interactions, where $\phi = 0.40, c_{21} = 0.05, c_{31} = 0.55, c_{32} = 0.12, c_{12} = 0.45, \eta = 0.70$, and γ is a parameter that varies between 0 and 0.9. The innovation scales are $(b_1, b_2, b_3, b_4, b_5) = (0.6, 0.5, 0.5, 0.6, 0.6)$. Expanding (VAR1) by rows gives (Eq. A3);

$$\begin{aligned} x_{1,t} &= \phi x_{1,t-1} + c_{21}x_{2,t-1} + c_{31}x_{3,t-1} + \gamma x_{4,t-1} + \varepsilon_{1,t}, \\ x_{2,t} &= \phi x_{2,t-1} + c_{12}x_{1,t-1} + c_{32}x_{3,t-1} + \gamma x_{4,t-1} + \varepsilon_{2,t}, \\ x_{3,t} &= \phi x_{3,t-1} + \varepsilon_{3,t}, \\ x_{4,t} &= \phi x_{4,t-1} + \eta x_{5,t-1} + \varepsilon_{4,t}, \\ x_{5,t} &= \phi x_{5,t-1} + \varepsilon_{5,t}. \end{aligned} \quad (\text{A3})$$

This structure separates the system into observable and hidden components. Only x_1, x_2, x_3 are assumed observable and are used for the IF estimation, whereas x_4 and x_5 act as hidden confounders. The causal design includes a bidirectional interaction between x_1 and x_2 , unidirectional influences $x_3 \rightarrow x_1$ and $x_3 \rightarrow x_2$, and a hidden driver x_4 that drive both x_1 and x_2 . A deeper, nested confounder x_5 drives x_4 (Fig. A1(a)). This nested confounding structure aims to mimic realistic Earth-system conditions where unobserved processes can influence, or even generate, additional confounders. To examine how confounding



strength affects IF estimation, we vary the parameter $\gamma \in \{0.0, 0.1, \dots, 0.9\}$, which controls the influence of the hidden
490 confounder x_4 on the observable variables x_1 and x_2 . For each γ , multiple independent realizations of length $N=3000$ are generated.

For every γ value, we compute the bivariate information flows $T_{1 \rightarrow 2}^{(bi)}$ and $T_{1 \rightarrow 3}^{(bi)}$ each using only the two variables involved, and the multivariate (conditioned) information flows $T_{1 \rightarrow 2|3}^{(mv)}$ and $T_{1 \rightarrow 3|2}^{(mv)}$ where one additional observed variable is included as a conditioning variable. To evaluate how conditioning alters the estimated causal strength, we compute the differential
495 information flows using Eq. (3) as (Eq. A4-A5);

$$\Delta IF_{1 \rightarrow 2} = T_{1 \rightarrow 2}^{(bi)} - T_{1 \rightarrow 2|3}^{(mv)} \quad (A4)$$

$$\Delta IF_{1 \rightarrow 3} = T_{1 \rightarrow 3}^{(bi)} - T_{1 \rightarrow 3|2}^{(mv)} \quad (A5)$$

Across 200 realizations, we compute bootstrap mean bands for each γ using $B=1000$ resamples, and percentile ribbons at the 1–99 % range. A significance mask marks ΔIF (or T) as significant when the bootstrap band excludes zero. These estimations
500 are repeated for $x_3 \rightarrow x_2$, as well to also quantify the influence of the mediator x_1 .

The results are summarized in Fig. A1, which illustrates the causal structure and clearly distinguishes observed and hidden components. The green region highlights the observable variables (x_1, x_2, x_3) used to compute IF. The grey regions contain the hidden confounders x_4 and x_5 , which influence the system but are deliberately excluded from the estimation. The hidden confounder x_4 injects shared variability into both x_1 and x_2 , while the additional variable x_5 introduces a deeper causal layer,
505 creating a confounder-of-a-confounder structure. As γ increases, the influence of the hidden confounder x_4 on the observed variables becomes stronger, amplifying the confounding pressure that cannot be removed through conditioning on observed variables alone. This ensures that the observable system is subjected to increasing and unresolvable confounding, allowing the experiment to test whether IF remains reliable under such challenging conditions.

Figure A1(b) shows that the IF from $x_1 \rightarrow x_3$ remain essentially zero across all γ values. This behavior is fully consistent with
510 the underlying system, which contains no direct causalities from x_1 to x_3 . Both the bivariate and multivariate IF estimates demonstrate that the presence of hidden confounders does not induce spurious causal inference in these couplings. In contrast, the causal pathway $x_1 \rightarrow x_2$ is consistently detected, although it strengthens as γ increases. The IF values for this pathway show a rise with increasing hidden confounder strength, reflecting the fact that x_4 amplifies the coupling between x_1 and x_2 since x_4 increases the feedback between x_1 and x_2 . Importantly, the bivariate and multivariate IF curves remain nearly
515 indistinguishable throughout the entire γ range, indicating that conditioning on the third observed variable x_3 provides only a negligible adjustment. The $x_3 \rightarrow x_2$ coupling also tests how IF responds to mediators (x_1). Figure A1(c) shows that x_1 does

not alter the inferred causal direction between x_3 and x_2 . This confirms that IF preserves directional fidelity under substantial hidden confounding, while still reflecting the influence of confounders and mediators (conditioners) on the estimated coupling strength.

Overall, this theoretical experiment demonstrates that LKIF retains directional fidelity under increasing and nested hidden confounding. True causal connections, such as $x_1 \rightarrow x_2$, are consistently recovered, while nonexistent connections remain near zero. This result is consistent with the findings in Vannitsem et al (2024).

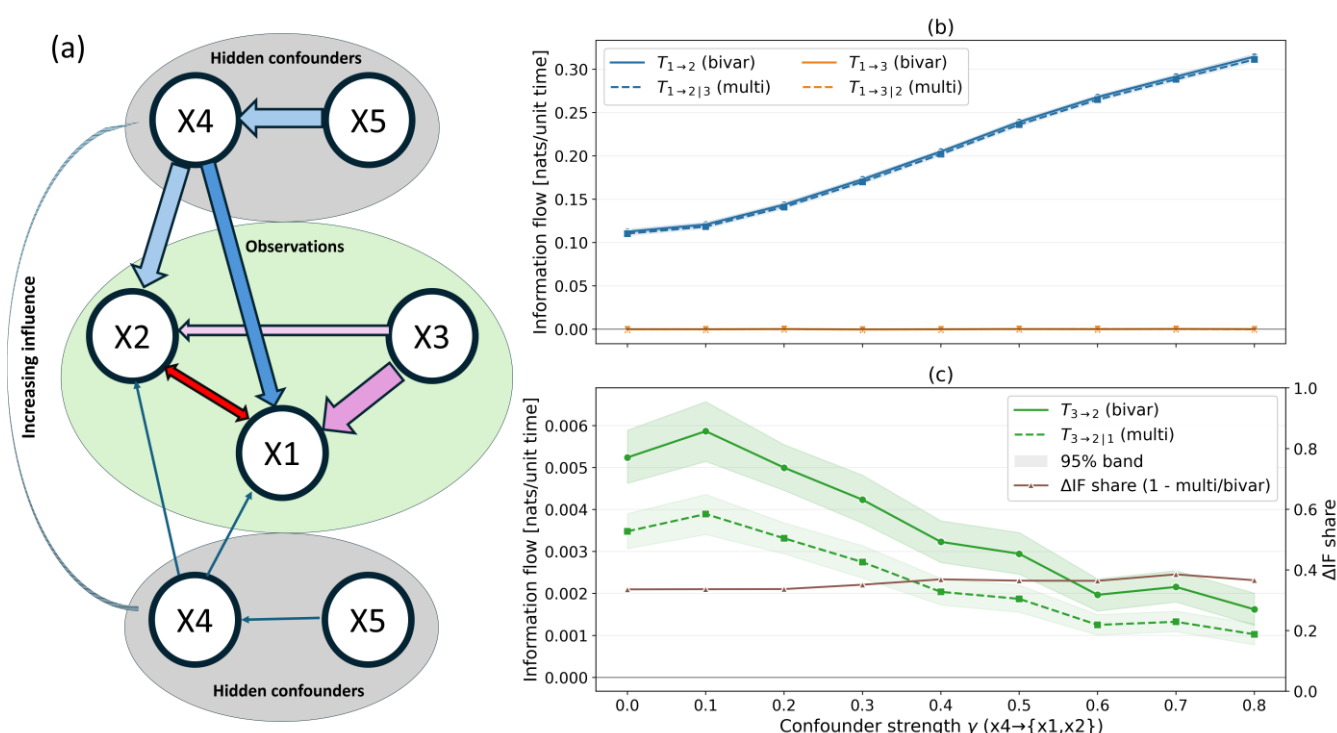


Figure A1: Toy-model experiment illustrating the effect of hidden confounders on Liang–Kleeman Information Flow (LKIF). (a) Causal graph for a five-variable system with three observed variables (x_1, x_2, x_3) and two hidden confounders (x_4, x_5). Directed arrows show the true causal pathways; blue arrows represent pathways originating from hidden confounders, the red arrow denotes the bidirectional coupling between x_1 and x_2 , and the pink arrows denote the causality of $x_3 \rightarrow x_1$ and $x_3 \rightarrow x_2$. Estimated bivariate (solid lines) and multivariate (dashed lines) IF for (b) $x_1 \rightarrow x_2$ and $x_1 \rightarrow x_3$ and (c) $x_3 \rightarrow x_2$ under increasing confounder strength γ , with the brown line showing the normalized differences (right y-axis). The shaded band shows the 95% confidence intervals.

Appendix B: Analysis Of Variance (ANOVA)



ANalysis Of Variance (ANOVA) was applied to the ΔIF values to quantify how their variability is structured across different hydroclimatic regimes. Monthly SM, VPD, T, and SSR were each partitioned into quartiles (Q1–Q4) using empirical quantiles. These quartile categories were then treated as factors in the ANOVA, which reports variance components across quartiles rather than individual quartile means. Three experimental designs were used:

535 (1) a two-way ANOVA: $SM_q \times VPD_q$.

(2) a three-way thermal ANOVA: $SM_q \times VPD_q \times T_q$.

(3) a three-way radiative ANOVA: $SM_q \times VPD_q \times SSR$.

These designs represent water-supply (SM), atmospheric-demand (VPD), and energy-constraint (Temperature or SSR) regimes.

540 For each design, ANOVA decomposed the variability in $|\Delta IF|$ according to the general multi-factor model (Eq. B1),

$$Y = \mu + \alpha i + \beta j + \gamma k + \delta l + (\alpha\beta)ij + (\alpha\gamma)ik + (\beta\gamma)jk + (\alpha\beta\gamma)ijk + \dots + \varepsilon ijkl, \quad (B1)$$

In this model, Y denotes the ΔIF values for each combination of SM, VPD, and T/SSR quartiles. The term μ is the grand mean, while αi , βj , γk and δl represent the main effects of SM, VPD, T, and SSR quartiles. The interaction terms $\alpha\beta ij$, $\alpha\gamma ik$, $\beta\gamma jk$, and $(\alpha\beta\gamma)ijk$ capture how combinations of these factors jointly modify ΔIF beyond their individual effects. The residual $\varepsilon ijkl$

545 accounts for unexplained variability.

In Eq. (B2), the total variability was partitioned into sums of squares using

$$SS_{Total} = \sum_{t=1}^N (y_t - \bar{y})^2 \quad (B2)$$

Here, y_t represents each ΔIF value, $\bar{y}$ is the overall mean across all ΔIF values, and SS_{Total} measures the total variability in ΔIF before attributing it to any factor or interaction.

550 In Eq. (B3),

$$SS_X = \sum_i n_i (\bar{y}_i - \bar{y})^2 \quad (B3)$$

SS_X quantifies the amount of ΔIF variability explained by a specific factor X (SM, VPD, temperature, SSR). Here, $\bar{y}_i$ is the mean ΔIF for level i of factor X , n_i is the number of observations in that level, and $\bar{y}$ is the overall mean. The same structure applies to interaction terms (e.g., $SS_{SM \times VPD}$), where the means $\bar{y}_{ij}$ correspond to pairs (or triples) of factor levels.



555 The residual variability is (Eq. B4),

$$SS_{Error} = SS_{Total} - \sum_X SS_X \quad (B4)$$

represents the portion of ΔIF not accounted for by any main factor or interaction term.

To characterize the strength of each regime effect, the bias-corrected omega-squared statistic was used (Eq. B5),

$$\omega_X^2 = \frac{SS_X - df_X MS_{Error}}{SS_{Total} + MS_{Error}} \quad (B5)$$

560 This equation defines omega-squared for factor X , which measures the proportion of the variance in ΔIF that is attributable to that factor after correcting for bias. SS_X is the sum of squares explained by factor X , and df_X is the degrees of freedom associated with it. MS_{Error} is the mean square of the residual error and equal to $MS_{Error} = SS_{Error} / df_{Error}$. SS_{Total} is the total sum of squares of ΔIF .

Omega-squared provides a bias-corrected estimate of the fraction of total ΔIF variability explained by factor X . Larger values
 565 of ω_X^2 indicate that the environmental regime represented by X plays a stronger role in shaping ΔIF .

The corresponding physically interpretable magnitude was given by the explained standard deviation (Eq. B6),

$$SD_X = \sigma_Y \sqrt{\omega_X^2} \quad (B6)$$

expressed in the same units as $|\Delta IF|$, where σ_Y is the standard deviation of ΔIF and ω_X^2 is the variance explained by factor X .
 Bootstrap resampling within each SM×VPD (or SM×VPD×T / SM×VPD×SSR) regime provided 95% confidence intervals
 570 for both ω^2 and SD .

Code and data availability. The ERA5 climate variable data are publicly available from the Copernicus Climate Data Store at <https://cds.climate.copernicus.eu/>. The GLASS GPP and LAI datasets (Liang et al., 2021) are accessible at www.glass.umd.edu. The scripts used to compute the rate of information transfer and to generate the figures presented in this study are available at (<https://github.com/FareehaSiddique/Conditioners-LKIF>).

575

Author contribution. FS, DFTH, and GW conceptualized and designed the study. FS and DFTH developed and implemented the computational workflow, performed the analyses, produced the figures, and interpreted the results. FS and DFTH wrote the manuscript with contributions from GW. DD and SV contributed to the methodological design and interpretation of the results. DD also provided feedback and suggestions to improve the figures. DD, SV, and GW reviewed and edited the
 580 manuscript. All authors reviewed the final version of the manuscript.



Competing interests. The authors declare that they have no conflict of interest.

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