

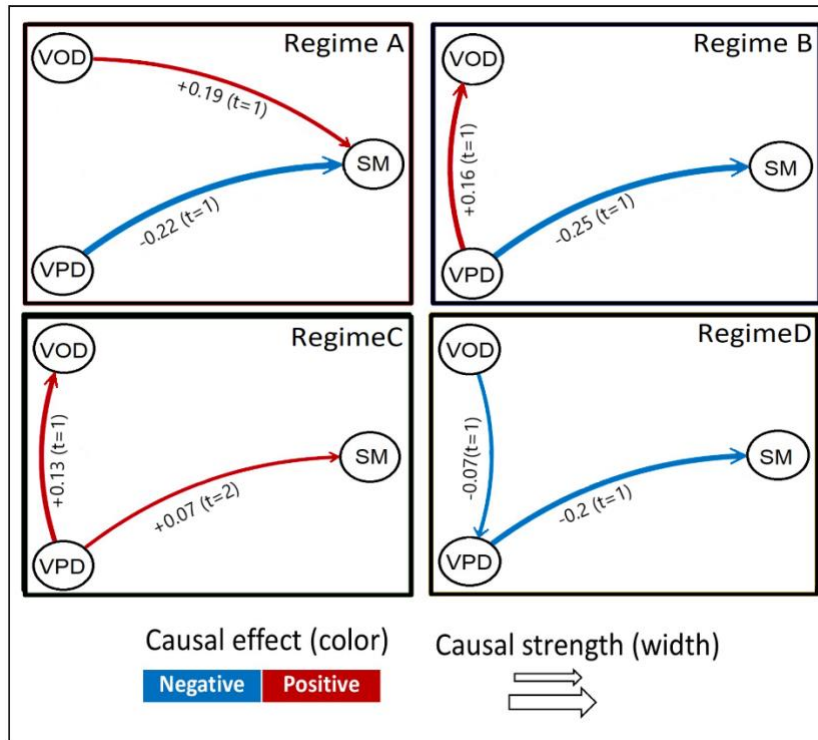


Figure S1: Directed acyclic graphs of lagged causal interactions for Regimes A-D. The graphs in each set show the causal network at different lag times ($t = 1, 2, 3$ days), with arrow color indicating the sign of the effect (red = positive; blue = negative), arrow width proportional to the strength of causation, and numerical labels showing the quantified strength of the link at each lag. This multi-lag representation reveals the time evolution of the feedbacks between soil moisture, VPD and VOD in grassland regimes.

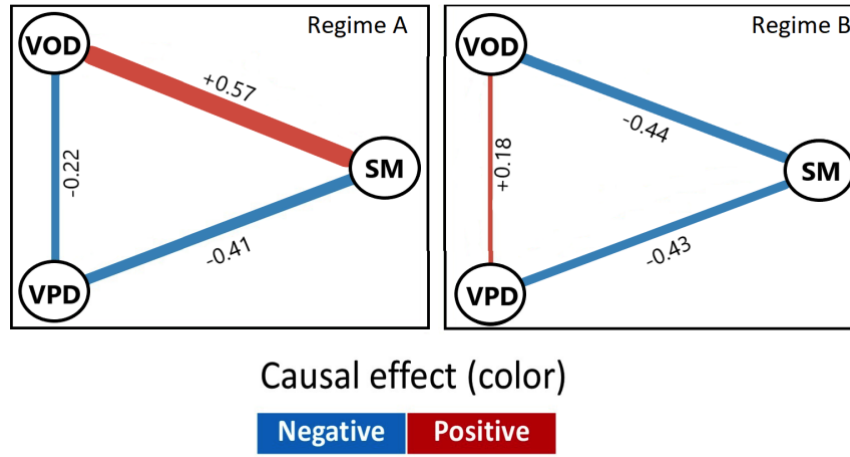


Figure S2: Covariate-conditioned causal structure of the core soil-moisture-vegetation-atmosphere coupling for (a) Regime A and (b) Regime B, from the expanded PCMCI model including additional conditioning variables of 30-day antecedent precipitation index (API), growing degree days (GDD) and incoming shortwave radiation (srad). For better visualization, only the three primary links between soil moisture (SM), vegetation optical depth (VOD) and vapor pressure deficit (VPD) are demonstrated. The diagnostic SM→VOD sign reversal between regimes remains after removing the effects of API, GDD and srad (Regime A: $\beta = +0.57$, Regime B: $\beta = -0.44$). The VPD→SM (A: -0.41 , B: -0.43) and VPD→VOD (A: -0.22 , B: $+0.18$) edges also remain. All displayed links remain significant, demonstrating that the basic SM–VPD–VOD coupling structure is not an artifact of confounding meteorological or energy-balance drivers.

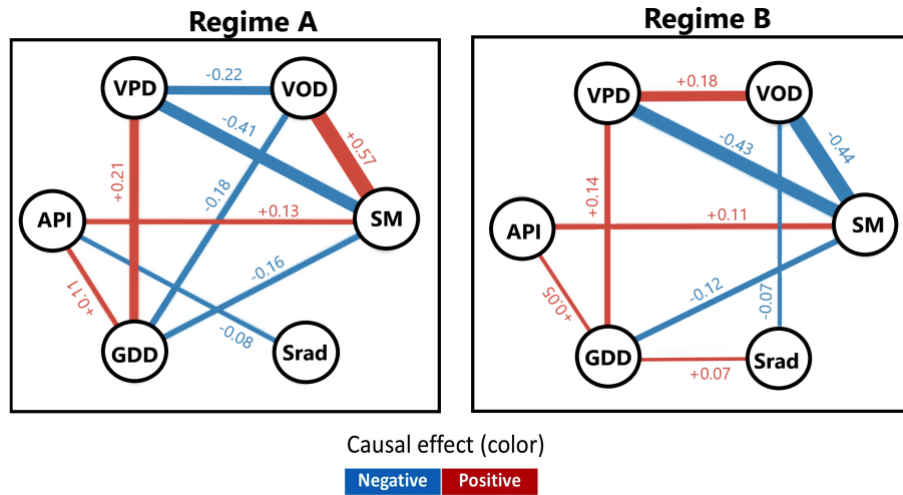


Figure S3: Full causal graph of the extended PCMCI model for (a) Regime A and (b) Regime B, showing all FDR significant ($q = 0.05$) causal links between soil moisture (SM), vegetation optical depth (VOD), vapor pressure deficit (VPD), the 30-day antecedent precipitation index (API), growing degree days (GDD), and incoming shortwave radiation (srad). The newly admitted covariates only add weak-to-moderate edges. The core SM→VOD, VPD→SM and VPD→VOD coefficients remain the same sign and near-identical magnitude as in the covariate-free model (Fig. 3) and in the SM–VPD–VOD-only view (Fig. S2). Therefore, the SM→VOD sign reversal between Regime A (+0.57) and Regime B (−0.44) remains the dominant causal signature separating the two pathways even when conditioned on preceding precipitation, thermal forcing and radiative forcing. The analysis was carried out on the 98.8% of pixels with complete covariate coverage (see Sects. 2.5 and 3.6).

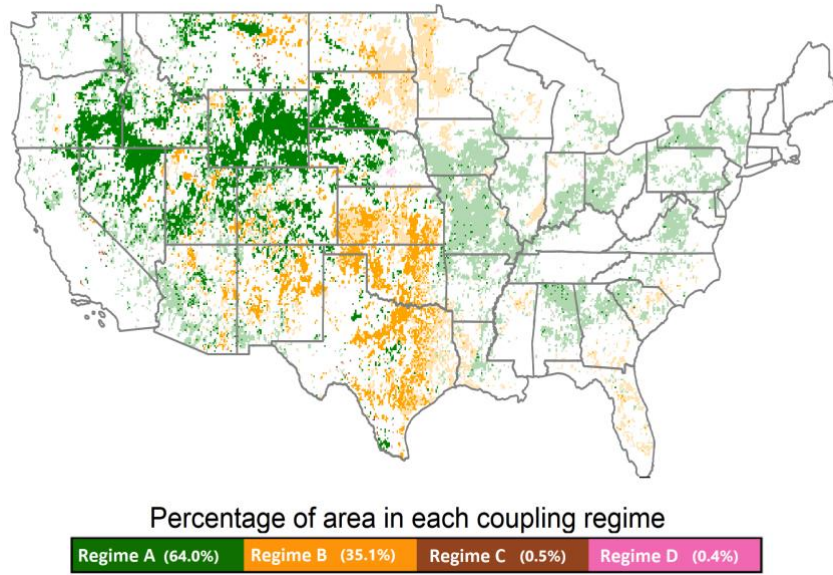


Figure S4: Coupling-regime map after conditioning on the candidate confounders API, GDD, and sradi. 98.8% of grassland pixels keep their original regime label, indicating the regimes are not artifacts of precipitation memory, thermal forcing, or radiative supply.

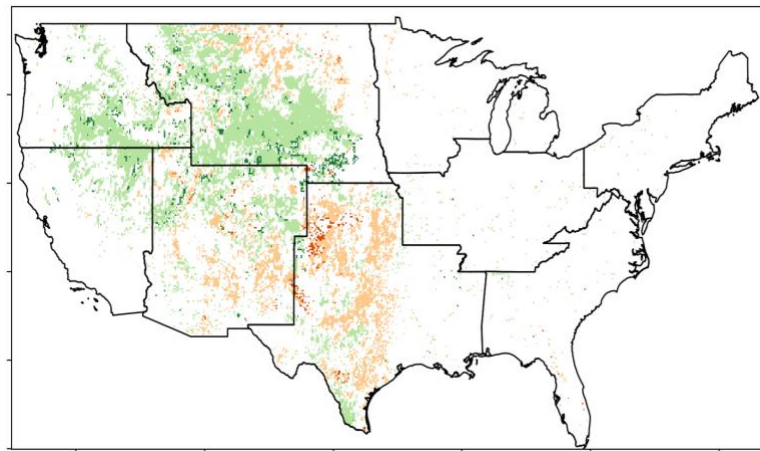


Figure S5: Spatial distribution of irrigation within grassland coupling regimes. Each grassland pixel in Regime A or B classified as rainfed ($\leq 10\%$ irrigation, light shading) or irrigated ($> 10\%$, dark shading). Irrigated pixels form a sparse, scattered minority in both regimes; $\sim 94\%$ of Regime B is rainfed.

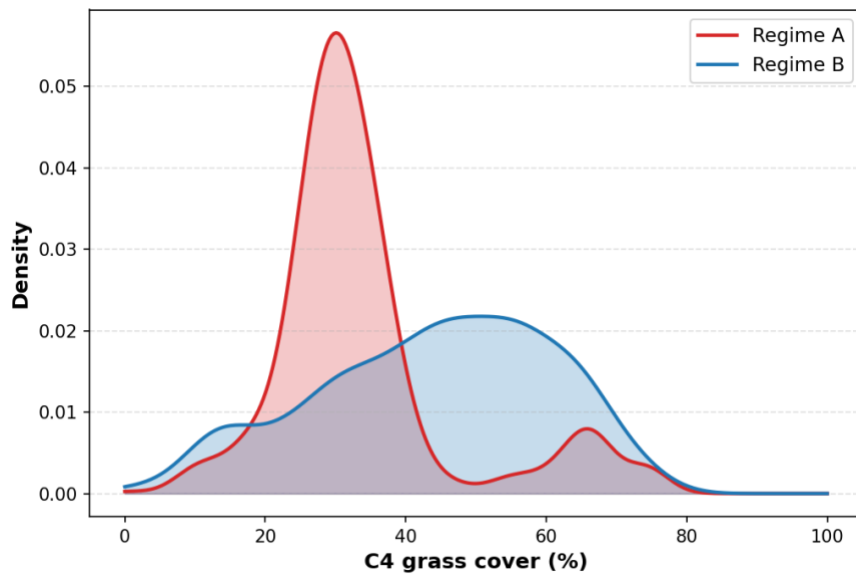


Figure S6: C4 grass cover distributions in high-purity natural grasslands for Regime A (red) and Regime B (blue). Regime B retains a markedly higher C4 fraction even after cropland-mixed and C4-crop pixels are removed.

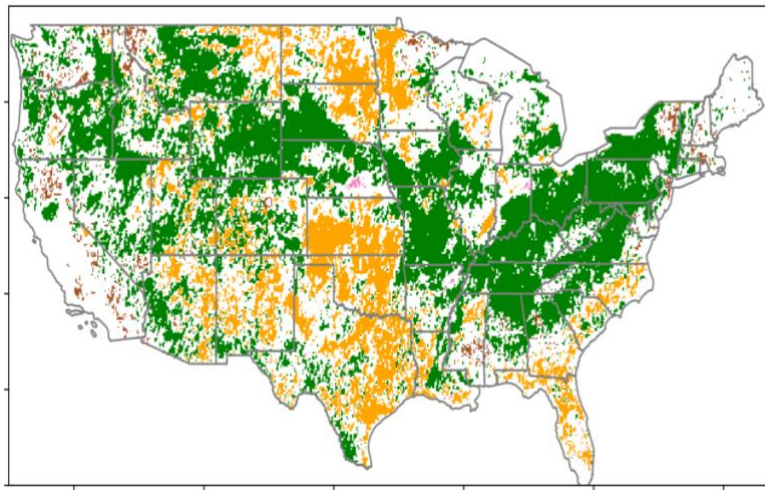


Figure S7: FDR-corrected ($q = 0.05$) coupling-regime map. The dominant spatial structure is preserved; only isolated, low-significance pixels are removed.

Table S1: Sensitivity of the C3/C4 grassland coupling-regime classification to the minimum drydown-segment length. Regime A and Regime B area fractions (% of the NLCD 2021 grassland mask over CONUS) from rerunning the full PCMCI pipeline with the minimum number of consecutive declining SMAP overpasses required to define a drydown segment set to 3, 4, and 5. The 4-overpass row corresponds to the value used in main manuscript. All other pre-processing steps and FDR-corrected significance threshold ($q = 0.05$) are the same across rows. The regime-area fractions change by ≤ 2.4 percentage points across the three drydown thresholds tested, and the six core PCMCI edges retain sign and near-identical magnitude.

Minimum drydown length	Regime A (%)	Regime B (%)
3	66.8	32.6
4	65.8	33.1
5	64.4	33.8

Table S2: Irrigation intensity within the two dominant grassland coupling regimes (LANID Landsat irrigation dataset; statistics over grassland pixels).

Regime	N pixels	Mean irrigation	Median	$\leq 10\%$ irrigated	$> 10\%$ irrigated
A (water-limited)	11,743	2.3%	0.000	92.7%	7.3%
B (SM↓ / VOD↑)	5,908	1.9%	0.001	94.0%	6.0%

Table S3: C4 fraction (Luo et al., 2024) in Regimes A and B on three nested domains: the full grassland domain, a high-purity natural-grassland subset (CDL grass $\geq 70\%$, cropland $\leq 20\%$, C4-crop $< 5\%$), and a pure rainfed natural-grassland subset (additionally excluding pixels with $> 10\%$ irrigation).

Domain	Median C4 A (%)	Median C4 B (%)	K–S D	p-value
Full grassland	26.0	40.5	0.42	1.8×10^{-13}
High-purity natural	30.9	45.6	0.507	2×10^{-95}
Pure rainfed natural	31.0	45.6	0.509	1×10^{-94}

Table S4: Causal coupling coefficients at the regime level with and without AR(1) infilling. Estimates are obtained on the native daily calendar with every infilled soil-moisture or VOD value flagged as missing, so that no reconstructed value enters the conditional-independence tests and a lag of τ retains the same meaning in days as in the with-infilling analysis (Sect. 2.2). The usable conditioning windows reduce from 630 to 554 in each regime, keeping 87.9% of the original windows. The regime-defining comparison is the SM–VOD rows. Change is shown relative to the with-infilling magnitude.

Regime	Link	With infilling	Observed only	Change	Sign	Dominant lag
A	SM–VOD	+0.590	+0.597	1.2%	retained	0, retained
A	SM–VPD	−0.430	−0.380	11.6%	retained	0, retained
A	VPD–VOD	−0.230	−0.210	8.7%	retained	0, retained
B	SM–VOD	−0.480	−0.494	2.9%	retained	0, retained
B	SM–VPD	−0.460	−0.410	10.9%	retained	0, retained
B	VPD–VOD	+0.200	+0.216	8.0%	retained	1, retained

Table S5: Sensitivity of the regime coupling to phenological constraint. The active season is defined for each pixel as the dates when the climatological VIIRS LAI exceeds the midpoint of that pixel’s warm-season range and is applied on a date-by-date basis so that gaps in the daily LAI record do not eliminate soil-moisture or VOD observations (Sect. 2.5). Each restriction is compared to contiguous random windows of equal length and number of usable samples; the z score represents the restricted SM–VOD coefficient relative to that control distribution and “outside” means a value outside the 5th–95th percentile range of the matched controls. The coefficients for Regime B are provided for the SM–VOD link.

Restriction	Retained steps	Regime B	Control	z (B)	z (A)	Assessment
$\geq 30\%$ of pixels active	411	−0.279	−0.238	−2.00	−0.09	B outside; A inside
$\geq 50\%$ of pixels active	194	−0.477	−0.208	−3.89	−0.64	B outside; A inside
Peak canopy, 1 Jul–15 Aug	322	−0.163	−0.205	+1.14	+0.07	Both inside

Table S6: Surface drying rates within the two dominant coupling regimes, computed over 720,639 drydown events in 17,651 grassland pixels (median 41 events per pixel). Each descriptor is reduced to a single value per pixel before comparison, and intervals are obtained by resampling pixels rather than events (Sect. 2.5). Rates are negative because soil moisture declines, so a positive A – B difference denotes faster surface drying in Regime B.

Descriptor	Regime A	Regime B	Difference (A – B)	95% interval
Mean rate (m ³ m ⁻³ d ⁻¹)	-0.00546	-0.01004	+0.00458	[+0.00435, +0.00478]
Early rate, first 3 d	-0.00945	-0.01362	+0.00417	[+0.00397, +0.00437]
Normalised early rate	-0.20084	-0.21020	+0.00936	[+0.00625, +0.01246]

Table S7: Surface drying-rate contrasts after stratification on initial soil moisture and mean VPD (5 × 5 strata), with within-stratum differences weighted by stratum size. Positive A – B values again denote faster surface drying in Regime B. Median surface sand fraction (OpenLandMap, 0–10 cm) is 42.5% in Regime A and 41.5% in Regime B, so the contrast is not attributable to soil texture.

Descriptor	Matched difference (A – B)	Strata compared
Mean rate	+0.00265	25
Early rate, first 3 d	+0.00126	25
Normalised early rate	+0.00403	25