Supplement of Geosci. Model Dev., 19, 4547–4565, 2026
https://doi.org/10.5194/gmd-19-4547-2026-supplement

Geoscientific Model Development
Open Access
EGU

Supplement of

A hybrid framework for the spin-up and initialization of distributed coupled ecohydrological-biogeochemical models

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Table S1. Examples of spin-up methods and applications used in ecohydrological and biogeochemical models across different spatial scales. The table summarizes the model name, spatial scale, and methodological approach. The category indicates whether the spin-up scheme was newly introduced or applied and eventually compared to other methods.

Source	Model	Scale	Description	Category
Zhan et al. (2003)	Simplified Simple Biosphere Model (SSiB)	Regional scale & Plot scale	Developed semi-analytical solution to stabilize and accelerate spin-up.	Introduced
Thornton & Rosenbloom (2005)	Biome-BGC Model	Plot scale	Introduced multiple spin-up acceleration methods: accelerated decomposition, N addition, General multivariate minimization methods.	Introduced
Basso et al. (2011)	DSSAT-CENTURY Model	Plot scale	Developed SOC pool initialization using site-specific land-use history.	Introduced
Hashimoto et al. (2011)	CENTURY v4 Model	Plot scale	Proposed slow-relaxation scaling of C/N pools during spin-up.	Introduced
Xia et al. (2012)	Community Atmosphere Biosphere Land Exchange Model (CABLE)	Global scale & Plot scale	Developed semi-analytical solution to accelerate coupled C-N model spin-up.	Introduced
Koven et al. (2013)	Community Land Model version 4 (CLM4)	Global scale	Introduced vertically resolved C-N model with pool-specific modified accelerated decomposition spin-up.	Introduced
Ng et al. (2014)	Community Land Model with Carbon-Nitrogen (CLM-CN)	Plot scale	Combined data assimilation with spin-up adjustments.	Introduced
Qu et al. (2018)	Terrestrial Ecosystem Model (TEM)	Plot scale	Developed analytical solution-based fast spin-up algorithm.	Introduced
Bruun & Jensen (2002)	Daisy Model	Plot scale	Compared equilibrium initialization vs. historical simulation.	Tested
Foereid et al. (2012)	DAYCENT Model	Plot scale	Tested steady-state and trend-fitting SOC initialization.	Tested
Nemo et al. (2017)	Rothamsted Carbon Model (RothC)	Plot scale	Evaluated C input adjustment and SOC fractionation methods.	Tested
Dimassi et al. (2018)	CENTURY v4.5 Model	Plot scale	Tested SOC initialization scenarios combining crop history and relaxation.	Tested
Lavin-Gullon et al. (2023)	Regional Climate Model (RCM)	Regional scale	Assessed spin-up time and variability in overlapping time slices.	Tested

Table S2. Mean absolute percentage error (MAPE) and normalized root mean squared error (NRMSE) of the random forest models trained using 40% of the tracked cells for predicting carbon and nitrogen pools in the original scenario. Both metrics are averaged over 10-fold cross-validation. Normalized mean absolute Shapley values are reported to indicate the relative importance of the six predictors.

Soil organic carbon pools	Robustness Metrics		Normalized mean absolute Shapley values					
	MAPE (%)	NRMSE	Elevation	Slope	Flow accumulation area	Curvature	Vegetation type	Sand content
Below-ground Litter Metabolic	3.09	0.05	22.4%	1.9%	6.7%	1.2%	65.4%	2.5%
Below-ground Litter Structural - Cellulose/Hemicellulose	5.99	0.04	10.4%	2.3%	2.8%	1.1%	81.8%	1.6%
Below-ground Litter Structura - Lignin	12.06	0.05	7.3%	2.2%	2.4%	1.2%	85.1%	1.7%
SOM-POC- lignin	11.49	0.05	6.2%	3.0%	3.4%	0.9%	85.1%	1.5%
SOM-POC -Cellulose/Hemicellulose	2.59	0.07	30.1%	10.2%	12.1%	1.7%	44.4%	1.4%
SOM-MOC	2.73	0.06	24.7%	7.2%	7.2%	1.6%	58.0%	1.3%
DOC - for bacteria	3.19	0.13	58.0%	14.3%	9.7%	3.6%	3.9%	10.5%
DOC - for fungi	2.66	0.13	58.9%	11.7%	9.5%	2.8%	5.2%	11.9%
Enzyme for decomposition of POC-Bact	2.93	0.07	18.2%	13.3%	16.4%	2.2%	43.4%	6.6%
Enzyme for decomposition of POC-Fung	2.49	0.07	16.1%	7.1%	8.2%	2.0%	61.3%	5.3%
Enzyme for decomposition of MOC-Bact	2.94	0.08	20.1%	12.5%	15.1%	2.7%	43.8%	5.8%
Enzyme for decomposition of MOC-Fung	2.48	0.07	16.7%	6.5%	7.7%	1.8%	62.0%	5.3%
Bacteria pool	5.28	0.08	12.4%	14.7%	16.7%	2.3%	52.2%	1.7%
Fungi saprotrophic	4.27	0.07	10.1%	8.5%	10.3%	1.5%	68.2%	1.5%
AM-Mycorrhizal - C	2.28	0.04	7.5%	1.3%	1.7%	0.7%	87.1%	1.7%
Soil organic nitrogen pools								
Nitrogen Above-ground Litter	4.39	0.04	12.6%	0.9%	1.5%	0.7%	82.9%	1.4%
Nitrogen Above-ground Woody	0.90	0.05	87.1%	4.7%	3.4%	2.2%	0.0%	2.6%
Nitrogen Below-ground Litter	3.02	0.06	20.3%	3.6%	10.2%	1.8%	60.3%	3.8%
Nitrogen SOM	1.52	0.07	35.9%	5.0%	6.1%	1.1%	50.4%	1.5%
Nitrogen Bacteria	5.20	0.08	11.2%	16.2%	17.2%	1.9%	51.7%	1.9%
Nitrogen Fungi	4.22	0.06	9.2%	8.9%	9.4%	1.6%	69.8%	1.2%
AM Mycorrhizal - N	2.21	0.04	9.6%	1.4%	1.3%	0.9%	85.0%	1.9%
Nitrogen Ione Ammonium NH4+	2.25	0.06	16.5%	3.7%	3.5%	1.4%	72.4%	2.5%
Nitrogen Nitrate NO3-	6.03	0.15	15.5%	17.2%	17.6%	2.8%	30.3%	16.5%
DON	6.98	0.12	32.5%	5.9%	14.1%	4.0%	29.1%	14.4%

Table S3. Comparison between soil organic carbon and nitrogen (SOC, SON) from the steady state condition with the biogeochemistry-only module (i.e., no coupled vegetation-soil biogeochemistry dynamics) and the reference steady state from the most comprehensive plot-scale spin-up (i.e., considering coupled vegetation-soil biogeochemistry dynamics) in the ten cells (see Fig. 2h in the main text). Information on vegetation cover and soil texture in these cells is also provided.

ID	Vege	Sand [%] Clay [%] Organic [%]	SOC [kg C/m^2]			SON [kg N/m^2]		
			Steady	Coevo.	Relative difference (%)	Steady	Coevo.	Relative difference (%)
1	Tree	40.9 27.5 6.8	12.51	13.51	-7.40	0.93	1.04	-10.58
2	Tree	42.0 24.9 9.0	10.46	12.31	-15.03	0.80	0.96	-16.67
3	Tree	42.5 24.3 8.6	10.36	11.94	-13.23	0.81	0.94	-13.83
4	Tree	42.5 25.9 7.2	11.90	13.74	-13.39	0.89	1.06	-16.04
5	Tree	39.5 25.9 8.3	11.53	12.90	-10.62	0.87	1.00	-13.00
6	Grass	41.7 26.5 6.7	6.70	8.42	-20.43	0.84	0.90	-6.67
7	Grass	41.3 26.9 7.1	6.41	8.00	-19.88	0.82	0.86	-4.65
8	Grass	40.4 27.9 8.5	6.32	7.76	-18.56	0.81	0.84	-3.57
9	Grass	40.1 26.7 7.2	6.91	8.29	-16.65	0.87	0.89	-2.25
10	Grass	41.6 26.5 6.3	6.73	8.36	-19.50	0.85	0.90	-5.56

Table S4. Jensen–Shannon divergence ($\times 10^{-4}$) between the probability density functions (PDFs) of soil organic carbon (SOC) and soil organic nitrogen (SON) from different percentages of tracked cells and those from the benchmark simulation across multiple simulation scenarios. Values in parentheses under the Random Soil scenario represent results obtained when clay content was included as an additional predictor in the random forest model.

Scenarios/Track cells [%]		10	20	40	60	80
Original	SOC	6.04	2.84	1.05	0.59	0.27
	SON	0.99	0.57	0.28	0.15	0.08
Random Veg	SOC	3.40	2.66	1.13	0.61	0.34
	SON	0.82	0.62	0.29	0.18	0.12
Homog. Veg	SOC	2.49	1.10	0.79	0.31	0.11
	SON	0.98	0.56	0.33	0.18	0.05
Random Soil	SOC	6659 (6.80)	24 (4.05)	21 (2.12)		
	SON	6725 (3.39)	16 (2.26)	2 (1.81)		
Homog. Soil	SOC	4.37	1.36	0.53		
	SON	0.50	0.24	0.12		
0.5 h_{max}	SOC	5.62	2.16	0.88		
	SON	0.98	0.57	0.25		
0.2 h_{max}	SOC	4.08	2.68	0.68		
	SON	0.70	0.37	0.18		

Table S5. Normalized mean absolute Shapley values of the seven predictors in random forest models trained using 40% of the tracked cells in the random soil scenario.

Soil organic carbon pools	Normalized mean absolute Shapley values						
	Elevation	Slope	Flow accumulation area	Curvature	Vegetation type	Sand content	Clay content
Below-ground Litter Metabolic	8.0%	1.9%	5.5%	1.2%	54.0%	3.4%	26.1%
Below-ground Litter Structural - Cellulose/Hemicellulose	5.3%	2.7%	2.8%	0.7%	81.0%	1.4%	6.0%
Below-ground Litter Structura - Lignin	3.8%	2.4%	2.4%	0.6%	84.7%	1.0%	5.0%
SOM-POC- lignin	2.9%	2.5%	2.4%	0.6%	75.8%	0.6%	15.2%
SOM-POC -Cellulose/Hemicellulose	4.9%	4.1%	5.3%	0.7%	21.0%	1.7%	62.4%
SOM-MOC	5.2%	3.6%	4.0%	0.7%	34.4%	1.3%	50.9%
DOC - for bacteria	19.5%	1.9%	1.9%	0.9%	0.8%	28.9%	46.0%
DOC - for fungi	21.1%	2.3%	1.9%	1.0%	0.6%	28.2%	44.9%
Enzyme for decomposition of POC-Bact	6.9%	5.5%	9.5%	2.2%	25.5%	14.4%	35.9%
Enzyme for decomposition of POC-Fung	7.4%	2.9%	4.6%	1.7%	41.4%	11.3%	30.7%
Enzyme for decomposition of MOC-Bact	6.6%	6.0%	10.9%	2.1%	25.2%	14.2%	35.0%
Enzyme for decomposition of MOC-Fung	7.1%	3.3%	4.7%	1.5%	42.1%	11.4%	30.0%
Bacteria pool	3.1%	10.9%	21.6%	2.4%	45.9%	2.2%	14.0%
Fungi saprotrophic	2.9%	5.8%	11.3%	1.7%	68.1%	0.9%	9.3%
AM-Mycorrhizal - C	5.8%	1.0%	1.0%	0.6%	83.3%	1.0%	7.3%
Soil organic nitrogen pools							
Nitrogen Above-ground Litter	5.8%	1.3%	2.1%	0.5%	61.1%	1.8%	27.6%
Nitrogen Above-ground Woody	88.2%	3.4%	3.6%	0.8%	0.0%	0.9%	3.2%
Nitrogen Below-ground Litter	5.9%	2.8%	7.9%	1.4%	28.9%	4.8%	48.2%
Nitrogen SOM	9.5%	2.3%	2.1%	0.6%	32.8%	1.8%	51.0%
Nitrogen Bacteria	3.3%	10.2%	20.9%	2.7%	47.9%	2.3%	12.8%
Nitrogen Fungi	2.7%	5.9%	10.6%	1.5%	69.2%	0.9%	9.1%
AM Mycorrhizal - N	5.0%	1.1%	0.9%	0.7%	83.7%	1.3%	7.3%
Nitrogen Ione Ammonium NH4+	7.3%	1.9%	1.7%	1.5%	67.5%	2.6%	17.6%
Nitrogen Nitrate NO3-	14.0%	7.7%	7.7%	2.3%	8.2%	8.4%	51.8%
DON	10.5%	8.0%	12.1%	2.4%	31.6%	23.6%	11.8%

Table S6. Wall-clock times for different components of the original and hybrid spin-up procedures. Results are shown for different fractions of tracked cells ($n = 10\%$, 20%, 40%, and 100%). In the 2D simulations, T_w denotes the wall-clock time required to simulate one year and N_y is the number of simulated years. For the tracked cell spin up, T_w represents the wall-clock time per tracked cell and N_{cell} denotes the number of tracked cells.

Computation Demand	Plot-initialization (9 years) [h]	2D simulation (T_w * N_y) [h]				Sum [h]
Original spin-up	0.11	2031 = (6.77*300)				2031.11
Hybrid spin-up with n=X%	Plot-initialization (9 years) [h]	2D simulation with tracking (T_w * N_y) [h]	Tracked cells spin up (T_w * N_{cell}) [h]	RF traning	Second 2D simulation [h]	Sum [h]
n=10%	0.11	75.33 = (8.37*9)	2.12= (0.0114*186)	Negligible	60.93	138.49
n=20%	0.11	90.90 = (10.1*9)	4.24 = (0.0114*372)	Negligible	60.93	156.18
n=40%	0.11	216.00 = (24*9)	8.48 = (0.0114*744)	Negligible	60.93	285.52
n=100%	0.11	433.53 = (48.17*9)	21.19 = (0.0114*1859)	Negligible	60.93	515.76

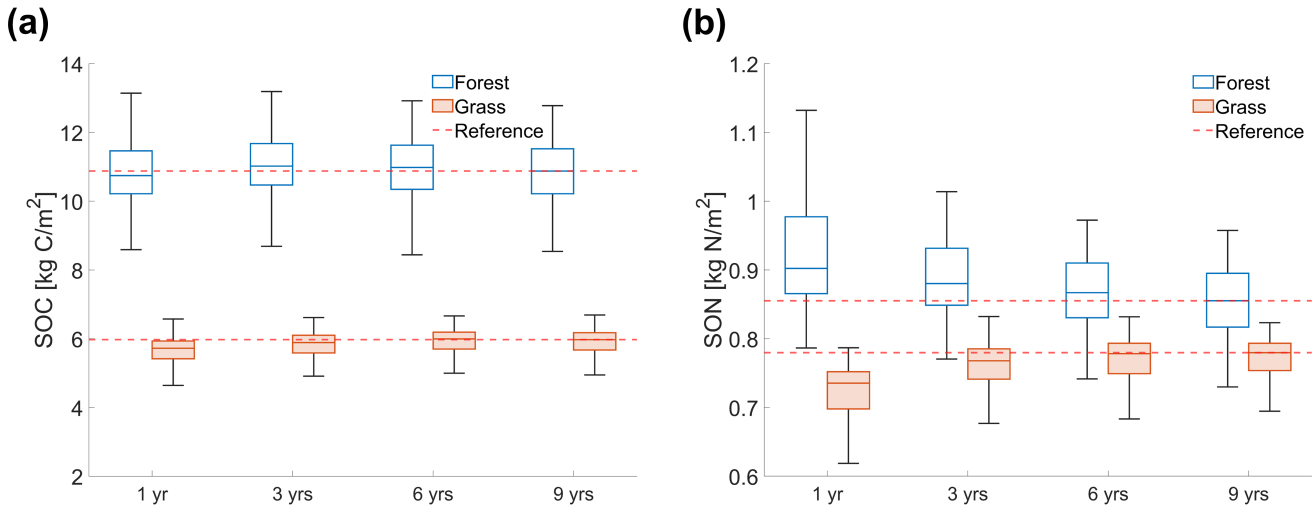

Figure S1. Comparison of steady state of (a) soil organic carbon (SOC) and (b) soil organic nitrogen (SON) using only the biogeochemistry module, with forcing and flux tracking periods of 1 year, 3 years, 6 years, and 9 years (reference). The forcing and flux tracking period is repeated to complete the 1000-year spin-up of the biogeochemistry module.

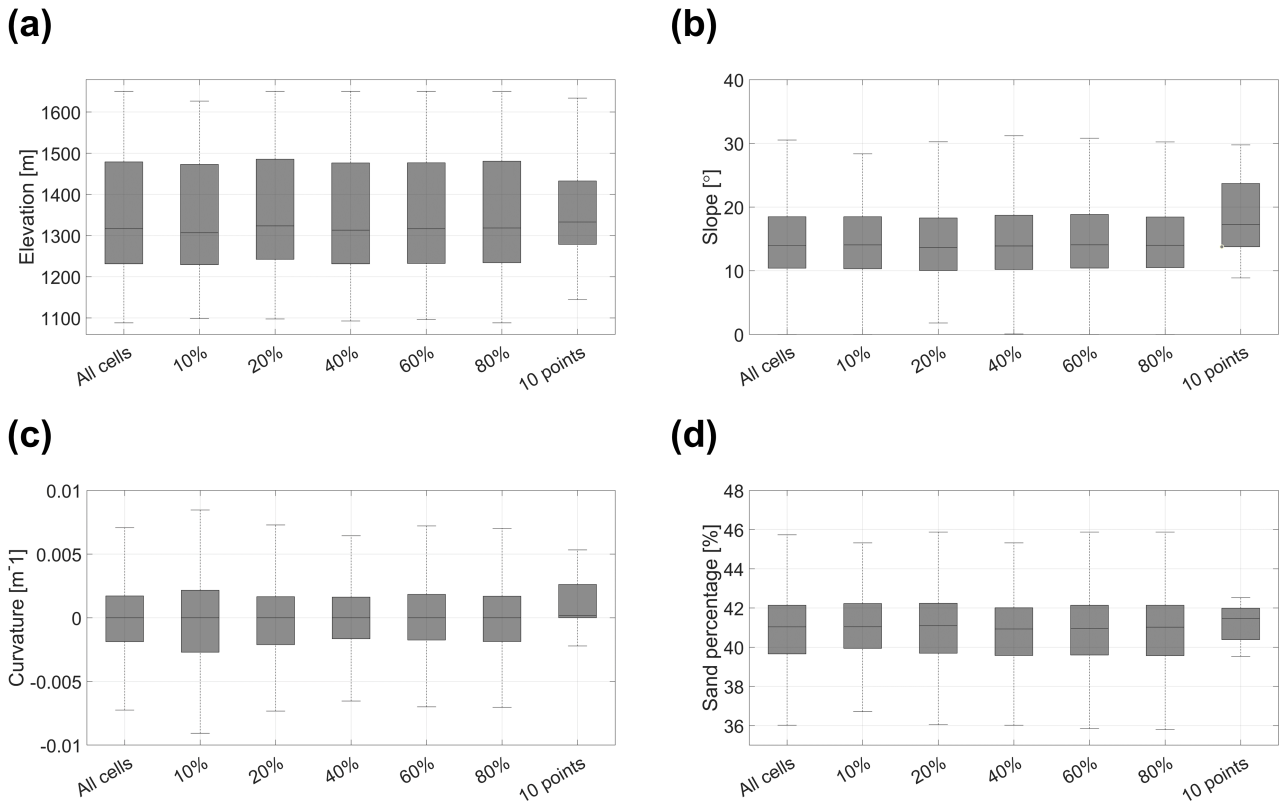

Figure S2. Distribution of topographic and soil attributes for all grid cells and selected subsets used for random forest model training. Panels show the distributions of (a) elevation, (b) slope, (c) curvature, and (d) sand percentage for all cells in the domain ("All cells"), different percentages of tracked training cells (10%–80%), and the 10 selected reference points for additional plot-scale simulation. The distributions indicate that the selected subsets preserve the key topographic and soil characteristics of the full domain.

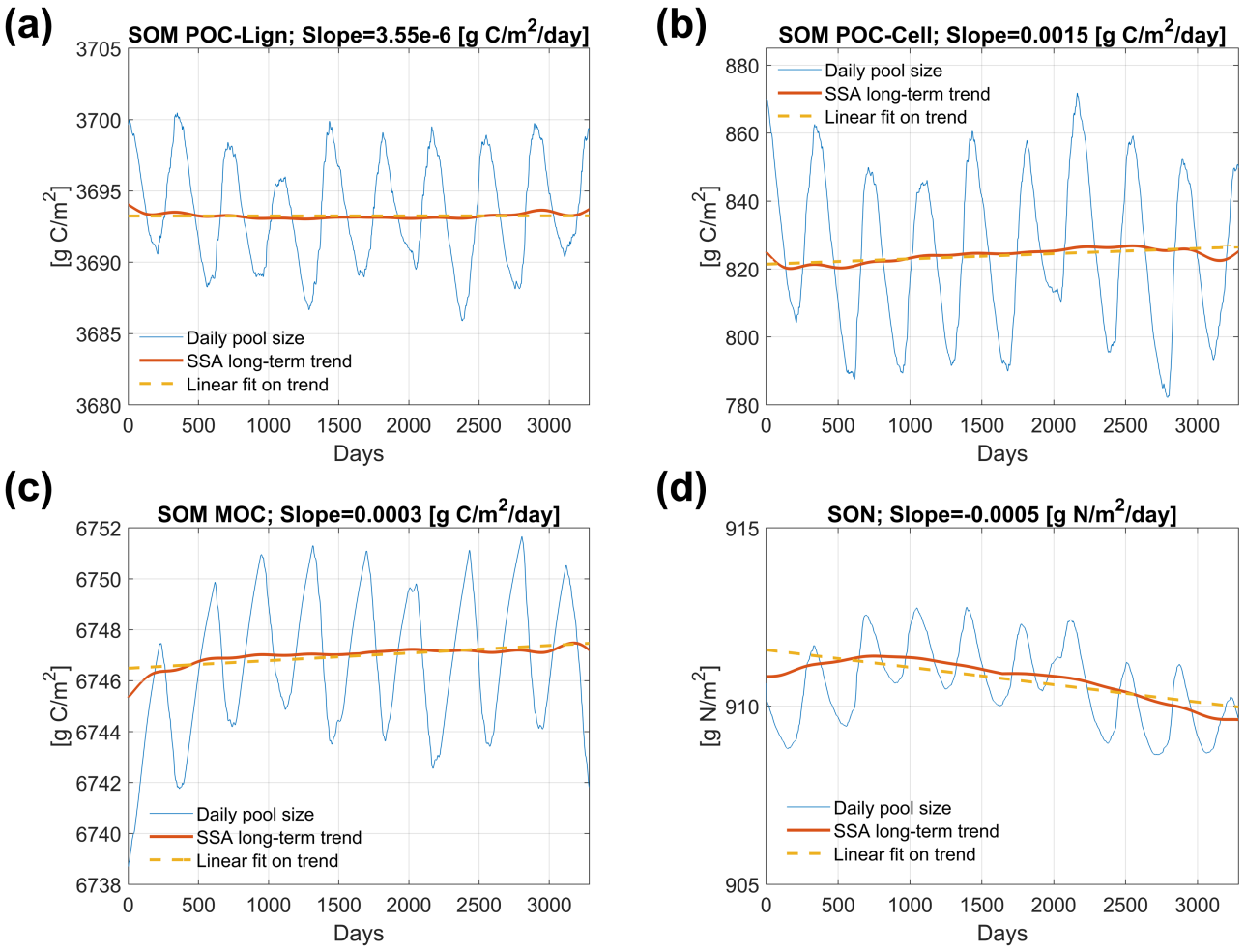

Figure S3. Time series of soil carbon and nitrogen pools during the 9-year coupled simulations for a representative grid cell. Long-term trends extracted using singular spectrum analysis (SSA), the corresponding linear fits, and the slopes (in gC $m^{-2}d^{-1}$ or gN $m^{-2}d^{-1}$) of the fitted trends are shown. Carbon pools include soil organic matter particulate organic carbon (SOM–POC) associated with lignin (SOM–POC–Lign; panel a) and cellulose/hemicellulose (SOM–POC–Cell; panel b), and mineral-associated organic carbon (SOM–MOC; panel c). Nitrogen pools include nitrogen in soil organic matter (SON; panel d). All pools are considered to have reached steady-state conditions.

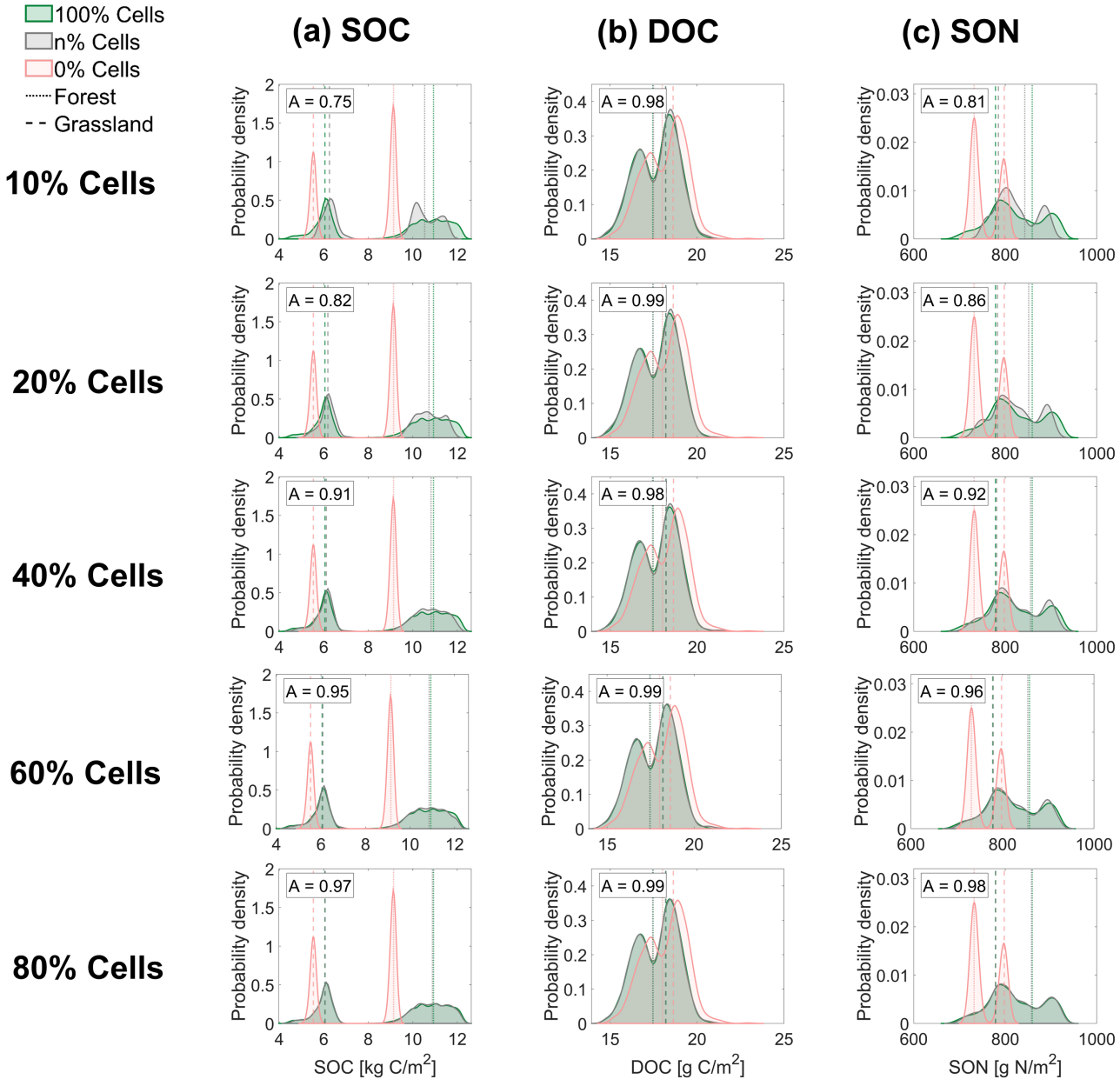

Figure S4. Probability density functions (PDFs) of (a) soil organic carbon (SOC), (b) dissolved organic carbon (DOC), and (c) soil organic nitrogen (SON) under different initialization settings using Random Forest (RF) with $n = 10\%$, 20%, 40%, 60%, and 80%. Each subplot compares the resulting distribution with those from the benchmark simulation using 100% of tracked cells (100% Cells) and from the simulation without cell tracking or RF (0% Cells). Shaded areas represent the overlapping region with the benchmark distribution. The overlap area between PDFs (A value) in each panel quantifies the similarity between the PDF and the benchmark. Dashed and dotted lines represent median values for grassland and forest areas, respectively.

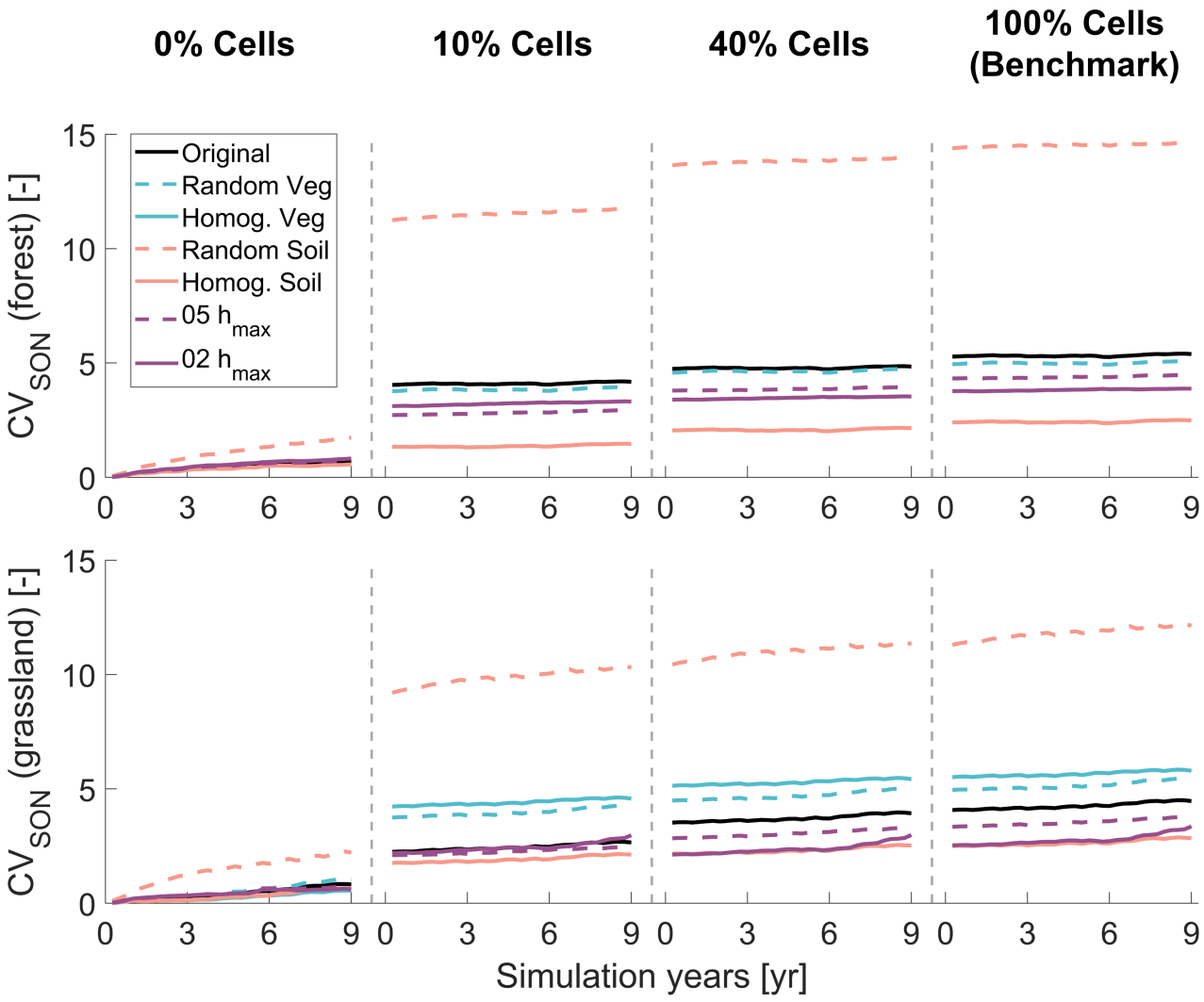

Figure S5. Temporal evolution of the coefficient of variation (CV) of soil organic nitrogen (SON) over a 9-year simulation period in forest (top) and grassland (bottom) under different initialization settings and simulation scenarios. Each column represents one initialization setting: no cell tracking and no random forest (0% Cells), $n = 10\%$ cells tracking and random forest (10% Cells), $n = 40\%$ cells tracking and random forest (40% Cells), and $n = 100\%$ cells tracking (100% Cells). Line colors and styles indicate results from different simulation scenarios, as shown in the legend.

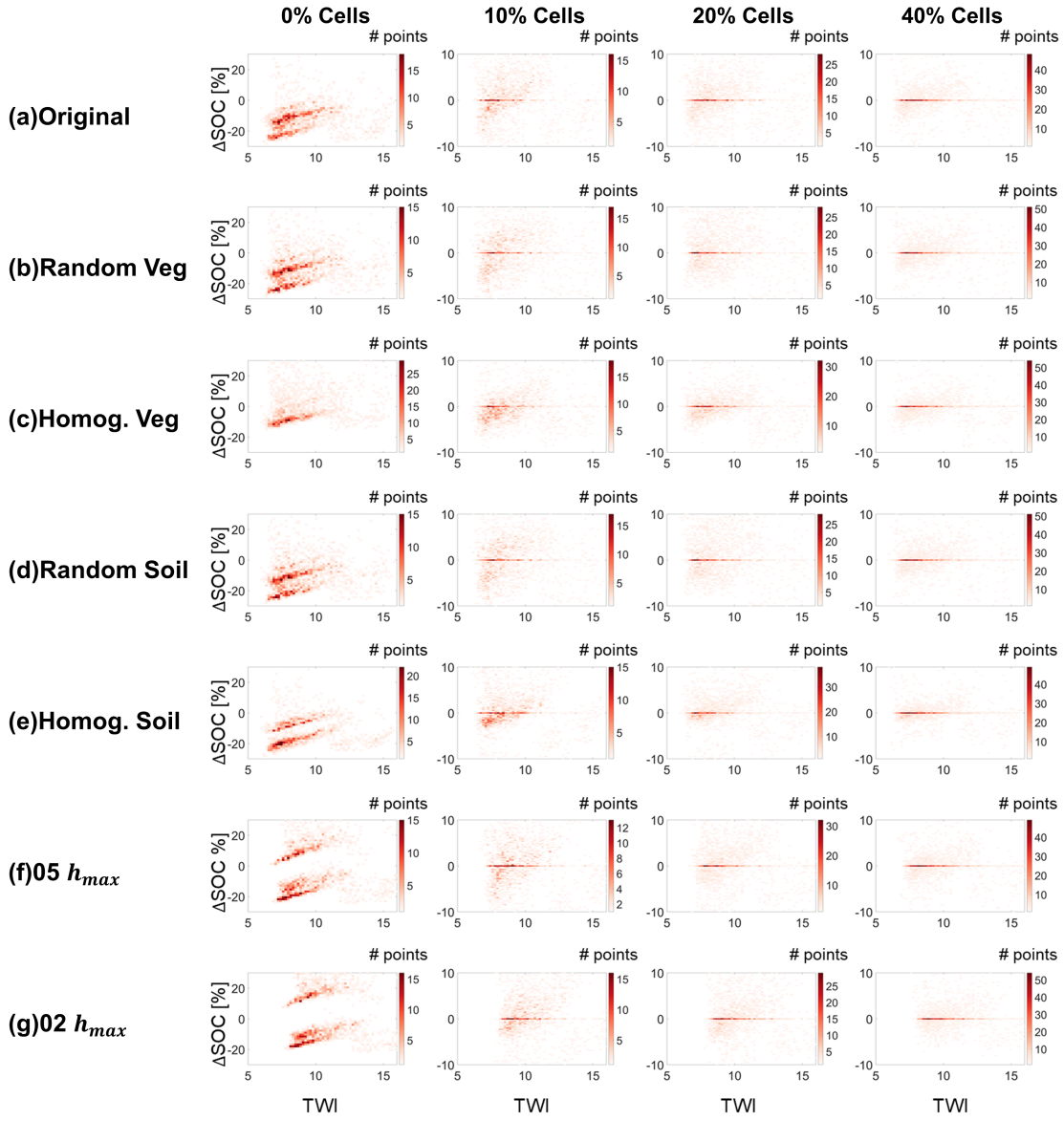

Figure S6. Density plots showing the relationship between relative SOC bias ($\Delta SOC = (SOC_{\text{simulation}} - SOC_{\text{benchmark}})/SOC_{\text{benchmark}}$), where $SOC_{\text{simulation}}$ represents results from different initialization settings, and the topographic wetness index (TWI) across all simulation scenarios. Results are shown for (a) Original, (b) Random Veg, (c) Homog. Veg, (d) Random Soil, (e) Homog. Soil, (f) 0.5 h_{max}, and (g) 0.2 h_{max} simulation scenarios. Columns represent different initialization settings: no cell tracking or RF ($n = 0\%$, 0% Cells), and RF-based initialization using $n = 10\%$, 20%, and 40% of tracked cells. The red color scale indicates the number of grid cells per bin.

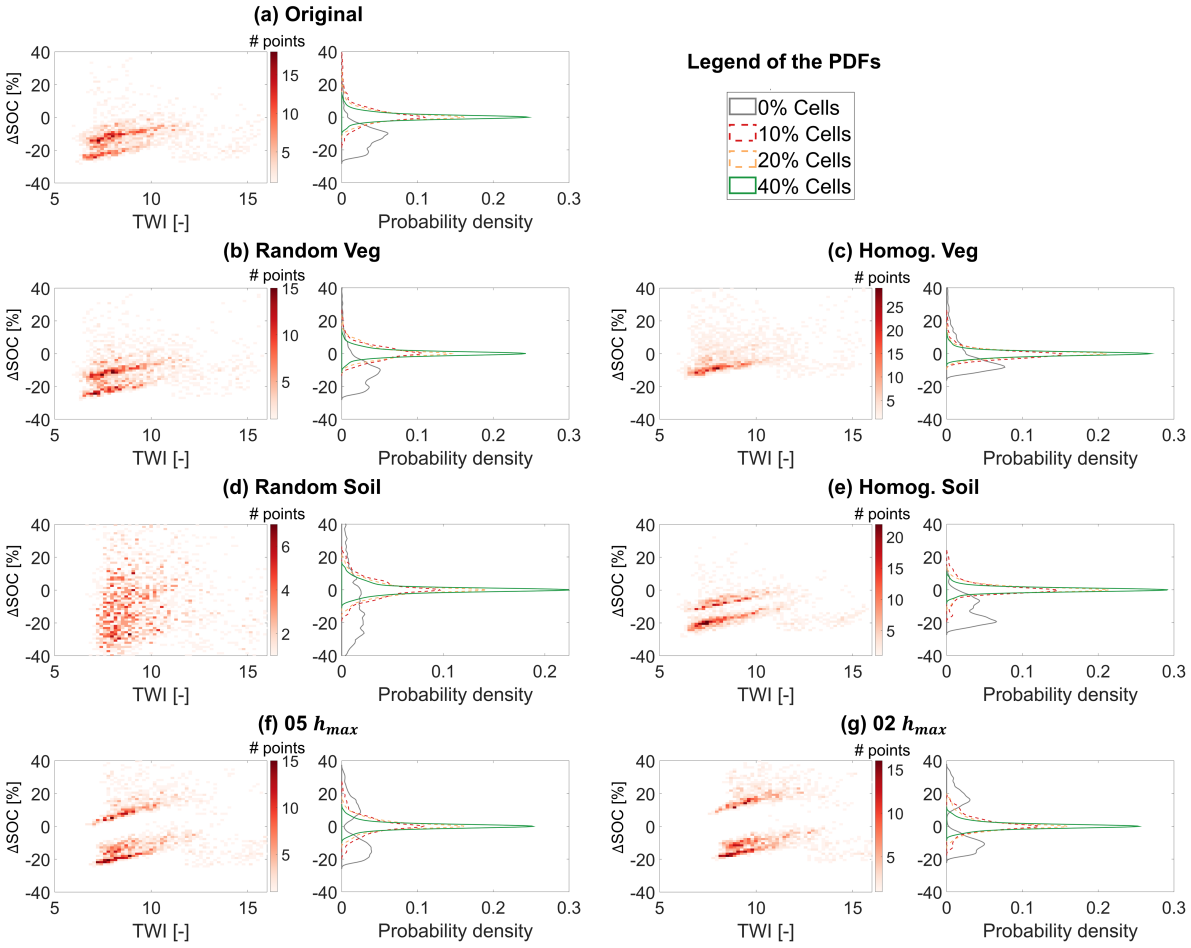

Figure S7. Density maps showing the relationship between SOC bias from the simulations without cell tracking and random forest ($n = 0\%$, 0% Cells) and topographic wetness index (TWI) across different simulation scenarios (left panels of each subfigure; $\Delta SOC = SOC_{simulation} - SOC_{benchmark}$). Probability density functions (PDFs) of ΔSOC from $n = 0\%$ simulation (in gray), and with RF-based initialization using $n = 10\%$ (red), 20% (yellow), and 40% (green) of tracked cells (right panels). Results are shown for (a) Original, (b) Random Veg, (c) Homog. Veg, (d) Random Soil, (e) Homog. Soil, (f) 0.5 h_{max}, and (g) 0.2 h_{max} simulation scenarios.

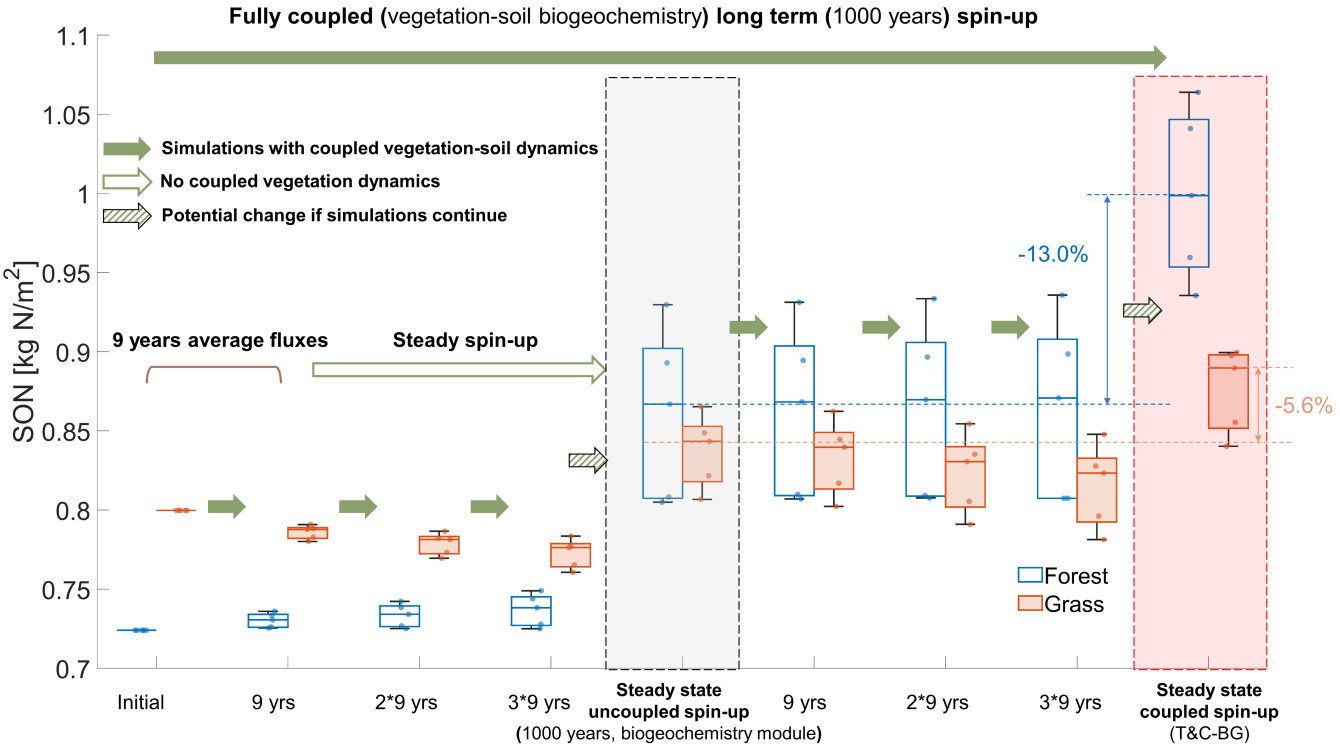

Figure S8. Evolution of soil organic nitrogen (SON) during different initialization schemes and simulation durations at 10 selected sites (Fig. 2h in the main text). Blue/orange boxplots represent forest/grassland sites. Arrows indicate simulation transitions between stages. The initial values (far left) are followed by 3 × 9-year simulations using the fully coupled T&C-BG model (solid green arrows). The average vegetation fluxes are extracted from the first 9 years to obtain a steady state condition with the biogeochemistry-only module (outlined green arrow, middle gray box). This is followed by three additional 9-year simulations. A comprehensive long-term spin-up using the fully coupled T&C-BG model (i.e., considering coupled vegetation and soil biogeochemical dynamics) is shown in the right red box. Striped arrows indicate the potential direction of SON change if coupled simulations continue beyond the current duration.

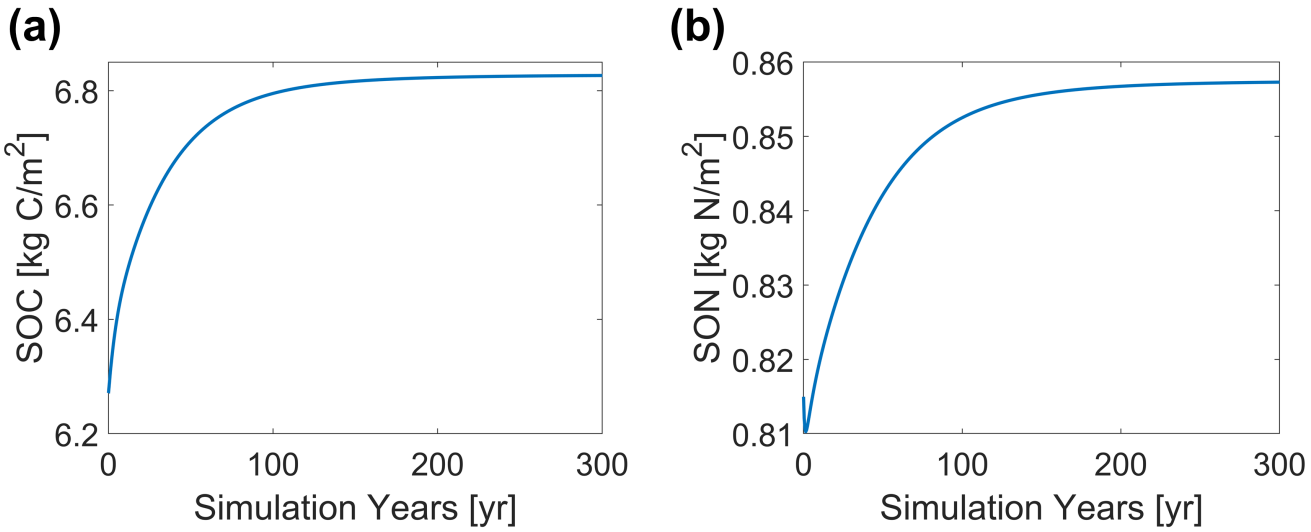

Figure S9. Example of temporal evolution of (a) soil organic carbon (SOC) and (b) soil organic nitrogen (SON) in a one-dimensional spin-up without coupled vegetation-soil biogeochemistry dynamics, based on repeated meteorological forcing at a representative grassland site in Erlenbach. SOC increases gradually over time, while SON initially declines before rising toward a steady state. The figure illustrates the slow convergence of soil carbon and nitrogen pools even under simplified conditions.

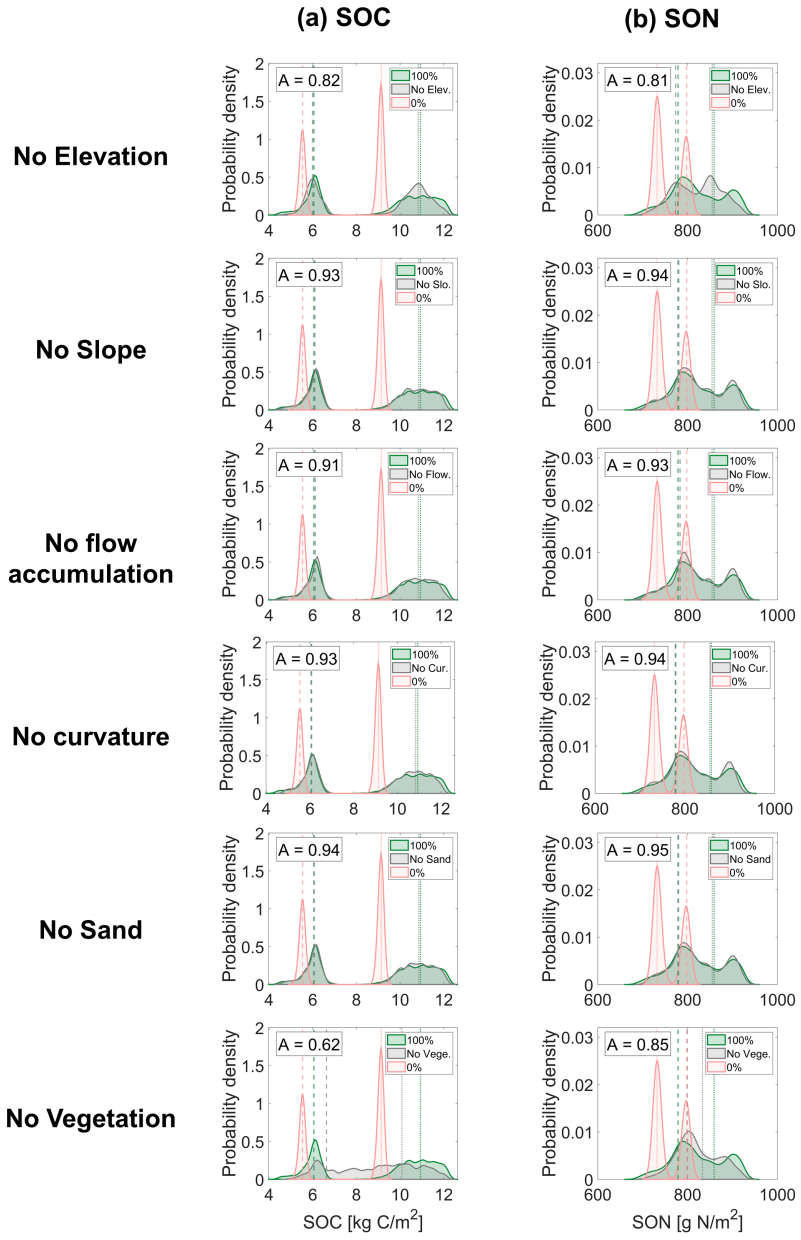

Figure S10. Sensitivity analysis of predictor importance in the Random Forest (RF) model for initializing spatial distributions of (a) soil organic carbon (SOC) and (b) soil organic nitrogen (SON) in the Erlenbach catchment. The analysis is conducted under the original simulation scenario using $n = 40\%$ of tracked cells for RF initialization. Each row shows the probability density functions (PDFs) of model outputs after removing one predictor from the RF training: elevation, slope, flow accumulation area, curvature, sand percentage, and vegetation type. Results are compared with the benchmark simulation using $n = 100\%$ tracked cells and the simulation without RF (No RF). Overlap area between PDFs (A value) quantifies the similarity between the RF-based distributions and the benchmark. Dashed and dotted lines represent median values for grassland and forest areas, respectively.

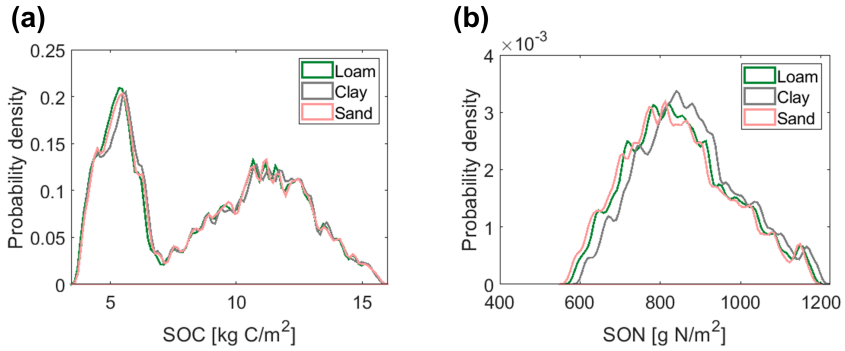

Figure S11. Probability density function of the spatial distribution of soil organic carbon (SOC) and soil organic nitrogen (SON) using three soil texture settings as initial conditions in step (a) in the initialization procedure. The spatial distribution results are the output of step (d) in Fig. 2 in the main text.

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