



8 **Abstract**

9 Understanding the influence of land surface heterogeneity on surface water and energy fluxes is  
10 crucial for modeling earth system variability and change. This study investigates the effects of four  
11 dominant heterogeneity sources on land surface modeling, including atmospheric forcing (ATM),  
12 soil properties (SOIL), land use and land cover (LULC), and topography (TOPO). Our analysis  
13 focused on their impacts on the partitioning of precipitation (P) into evapotranspiration (ET) and  
14 runoff (R), partitioning of net radiation into sensible heat and latent heat, and corresponding water  
15 and energy fluxes. An initial set of 16 experiments were performed over the continental U.S.  
16 (CONUS) using the E3SM land model (ELMv1) with different combinations of heterogeneous  
17 and homogeneous datasets. The Sobol' total and first-order sensitivity indices were utilized to  
18 quantify the relative importance of the four heterogeneity sources. Sobol' total sensitivity index  
19 measures the total heterogeneity effects induced by a given heterogeneity source, consisting of the  
20 contribution from its own heterogeneity (i.e., the first-order index) and its interactions with other  
21 heterogeneity sources. ATM and LULC are the most dominant heterogeneity sources in  
22 determining spatial variability of water and energy partitioning, mainly contributed by their own  
23 heterogeneity and slightly contributed by their interactions with other heterogeneity sources. Their  
24 heterogeneity effects are complementary both spatially and temporally. The overall impacts of  
25 SOIL and TOPO are negligible, except TOPO dominates the spatial variability of R/P across the  
26 transitional climate zone between the arid western and humid eastern CONUS. Accounting for  
27 more heterogeneity sources improves the simulated spatial variability of water and energy fluxes  
28 when compared with ERA5-Land reanalysis dataset. An additional set of 13 experiments identified  
29 the most critical components within each heterogeneity source, which are precipitation,

- 30 temperature and longwave radiation for ATM, soil texture and soil color for SOIL, and maximum
- 31 fractional saturated area parameter for TOPO.

32 **1. Introduction**

33 **Land surface heterogeneity plays a critical role in the terrestrial water, energy, and**  
34 **biogeochemical cycles from local to continental and global scales** (Giorgi and Avissar, 1997;  
35 Chaney et al., 2018; Zhou et al., 2019; Liu et al., 2017). As the land component of global Earth  
36 System Models (ESMs) and Regional Climate Models (RCMs), land surface models (LSMs) are  
37 used to simulate the exchange of momentum, energy, water, and carbon between land and  
38 atmosphere. LSMs have been widely utilized in studies focused on climate projection, weather  
39 forecast, flood and drought forecast, and water resources management (Clark et al., 2015;  
40 Lawrence et al., 2019). At the resolutions typically applied in ESMs and RCMs, LSMs have  
41 limited ability to resolve land surface heterogeneity to skillfully represent its impacts on the surface  
42 fluxes and subsequent effects on earth system and climate simulations through land-atmosphere  
43 interactions. Singh et al. (2015) demonstrated that increasingly capturing topography and soil  
44 texture heterogeneity at finer resolutions improves the land surface modeling of soil moisture,  
45 terrestrial water storage anomaly, sensible heat, and snow water equivalent. Therefore, better  
46 representing spatial heterogeneity in LSMs may be crucial to reliably simulate water and energy  
47 exchange between land and atmosphere (Essery et al., 2003; Jr. et al., 2017; Fan et al., 2019; Fisher  
48 and Koven, 2020).

49  
50 **Several approaches have been developed to resolve land surface heterogeneity in LSMs.** The  
51 most common class of method is the tile approach that subdivides each grid into several tiles to  
52 account for heterogeneous surface properties (Avissar and Pielke, 1989). The Community Land  
53 Model version 5 (CLM5) and the Energy Exascale Earth System Model (E3SM) land model (ELM)  
54 utilize a nested subgrid hierarchy in which each grid cell is composed of multiple land units, soil



55 columns, and plant functional types. Tesfa et al. (2017; 2020) developed a topography-based  
56 subgrid structure based on topographic properties such as surface elevation, slope, and aspect to  
57 better represent topographic heterogeneity in ELM. Swenson et al. (2019) introduced hillslope  
58 hydrology in CLM5 where each grid cell is decomposed into one or more multicolumn hillslopes.  
59 The second class of method to account for land surface heterogeneity is called the "continuous  
60 approach" in which subgrid heterogeneity is described via analytical or empirical probability  
61 density functions (PDFs) instead of dividing a grid cell into subgrid units. For example, He et al.  
62 (2021) developed the Fokker-Planck Equation subgrid snow model in the Rapid Update Cycle  
63 Land-Surface Model, which uses dynamic PDFs to represent the variability of snow in each grid  
64 cell. The third class of method to better account for land surface heterogeneity is by developing  
65 parameterizations for subgrid processes. For example, Hao et al. (2021) implemented a sub-grid  
66 topographic parameterization in the ELM to represent topographic effects on insolation, including  
67 the shadow effects and multi-scattering between adjacent terrains. Besides these three classes of  
68 approach dealing with subgrid heterogeneity, the fourth class is to directly increase the grid  
69 resolution. Previous studies have demonstrated the benefits of increasing resolution in simulating  
70 precipitation, temperature, and related extreme events over multiple spatial scales (Torma et al.,  
71 2015; Lindstedt et al., 2015; Cuesta-Valero et al., 2020; Koster et al., 2002; Vegas-Cañas et al.,  
72 2020; Rummukainen, 2016). The proposed hyperresolution land surface modeling by Wood et al.  
73 (2011) to model land surface processes at a horizontal resolution of 1 km globally and 100 m or  
74 finer continentally or regionally has been gaining attention as supported by increasing availability  
75 of high-performance computing resources (Singh et al., 2015; Rouf et al., 2021; Ko et al., 2019;  
76 Xue et al., 2021; Yuan et al., 2018; Chaney et al., 2016; Naz et al., 2018; Vergopolan et al., 2020;  
77 Garnaud et al., 2016; Bierkens et al., 2014).

78

79 **There are several heterogeneity sources in LSMs but their impact on water and energy**

80 **simulations at different spatial resolutions has not been systematically examined.** Four types

81 of heterogeneity sources are commonly categorized in land surface modeling, including

82 atmospheric forcing, soil properties, land use and land cover, and topography characteristics

83 (Singh et al., 2015; Ji et al., 2017). Singh et al. (2015) showed that including more detailed

84 heterogeneity of soil and topography at high resolutions improved the water and energy

85 simulations over the Southwestern U.S. Xue et al. (2021) demonstrated that simulations over the

86 High Mountain Asia region driven by high-resolution atmospheric forcing generally outperform

87 simulations that used coarse-resolution atmospheric forcing. Simon et al. (2020) investigated the

88 impacts of different heterogeneity sources (e.g., river routing and subsurface flow, soil type, land

89 cover, and forcing meteorology) on coupled simulations using the Weather Research and

90 Forecasting (WRF) model. They found that heterogeneous meteorology is the primary driver for

91 the simulations of energy fluxes, cloud production, and turbulent kinetic energy. Chaney et al.

92 (2016) conducted high-resolution simulations over a humid watershed and found that topography

93 and soils are the main drivers of spatial heterogeneity of soil moisture. However, these studies

94 generally focused either solely on one or a few heterogeneity sources, or were conducted over

95 small domains with limited climate and hydrologic variations. Therefore, a comprehensive

96 assessment of the contribution of different heterogeneity sources to heterogeneity in energy and

97 water fluxes simulated by LSMs at continental scales is needed.

98

99 **The relative importance of heterogeneity sources on LSM simulations can be quantified by**

100 **sensitivity analysis (SA), which has been commonly used to study parametric uncertainty**

101 (Saltelli, 2002). In a quantitative sensitivity analysis, the assessed factors could include model  
102 parameters as well as any other types of uncertainty induced by varying the input data (Saltelli et  
103 al., 2019). The Sobol' SA is a variance-based SA approach and has been widely utilized by the  
104 land surface modeling community (Rosolem et al., 2012; Nossent et al., 2011; Li et al., 2013b).  
105 The most common application is the assessment of model parameters importance. Cuntz et al.  
106 (2016) comprehensively assessed the sensitivities of the Noah-MP land surface model to selected  
107 parameters over 12 U.S. basins. This method is also utilized to quantify the sensitivity of model  
108 outputs to the choice of parameterization schemes. Dai et al. (2017) proposed a method based on  
109 Sobol' variance analysis to conduct SA while simultaneously considering parameterizations and  
110 parameters. Zheng et al. (2019) utilized the Sobol' method to quantify the sensitivity of  
111 evapotranspiration and runoff to different parameterizations in the Noah-MP land surface model  
112 over the CONUS. Given the demonstrated usefulness of the Sobol' sensitivity analysis method, it  
113 can be applied to quantify the relative importance of different heterogeneity sources on land  
114 surface water and energy simulations.

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116 **The overarching goal of this paper is to determine the relative importance of different**  
117 **heterogeneity sources on the spatial variability of simulated water and energy partitioning**  
118 **over CONUS.** The four heterogeneity sources considered in this study are atmospheric forcing  
119 (ATM), soil properties (SOIL), land use and land cover (LULC), and topography (TOPO). Our  
120 analysis focuses on their impacts on the water partitioning of precipitation into evapotranspiration  
121 and runoff, the energy partitioning of net radiation into sensible heat and latent heat, and their  
122 corresponding fluxes. ELMv1 is used as the model testbed. Two sets of experiments are conducted  
123 with different combinations of homogeneous and heterogeneous inputs. A set of 16 experiments

124 are used to assess the impacts of the four heterogeneity sources on water and energy partitioning  
125 using the Sobol' sensitivity analysis method. Subsequently, another set of 13 experiments are  
126 conducted to analyze the heterogeneity effects from each component of atmospheric forcing, soil  
127 properties, and topography. The remaining structure of this paper is organized as follows. Section  
128 2 describes ELM, data processing, experimental design, and analysis method. Results are  
129 examined in section 3, followed by discussions in section 4 and conclusions in section 5.

130

## 131 **2. Methodology**

### 132 **2.1 ELM overview**

133 The E3SM is a newly developed state-of-the-science Earth system model by the U.S. Department  
134 of Energy (Caldwell et al., 2019; Leung et al., 2020). ELMv1 started from the Community Land  
135 Model version 4.5 (CLM4.5; Oleson et al., 2013) and now includes more recently developed  
136 representations of soil hydrology and biogeochemistry, riverine water, energy and  
137 biogeochemistry, water management (Li et al., 2013a; Tesfa et al., 2014; Bisht et al., 2018; Yang  
138 et al., 2019; Zhou et al., 2020).

139

### 140 **2.2 ELM inputs**

#### 141 **2.2.1 Heterogeneity sources**

142 ATM forcing for ELM consists of seven surface meteorological variables, including precipitation  
143 (PRCP), air temperature (TEMP), specific humidity (HUMD), shortwave radiation (SRAD),  
144 longwave radiation (LRAD), wind speed (WIND), and air pressure (PRES). Atmospheric forcing  
145 from the North American Land Data Assimilation System phase 2 (NLDAS) is used in this study  
146 (Xia et al., 2012b, a). SOIL consists of soil texture (STEX), organic matter content (SORG), and  
147 soil color (SCOL). STEX and SORG determine soil thermal and hydrologic properties, while

148 SCOL regulates the soil albedo and hence surface energy related processes. LULC consists of the  
 149 glacier, lake, and urban fractions, the fractional cover of each plant functional type (PFT), and  
 150 monthly leaf area index (LAI) and stem area index (SAI) for each PFT. The LULC datasets at  
 151  $0.05^\circ \times 0.05^\circ$  developed by Ke et al. (2012) are used in this study. TOPO consists of the standard  
 152 deviation of elevation (SD\_ELV), maximum fractional saturated area (Fmax), and topography  
 153 slope. TOPO is used in snow cover parameterization, surface runoff generation and infiltration.  
 154 SOIL and TOPO datasets are obtained from the NCAR dataset pool for CLM5 (Lawrence et al.,  
 155 2019; Lawrence and Chase, 2007; Bonan et al., 2002; Batjes, 2009; Hugelius et al., 2013;  
 156 Lawrence and Slater, 2008). Table 1 summarizes these heterogeneity components and resolutions  
 157 of the source data. All datasets were prepared over the entire CONUS.

158 Table 1 Summary of heterogeneity sources in ELM model inputs

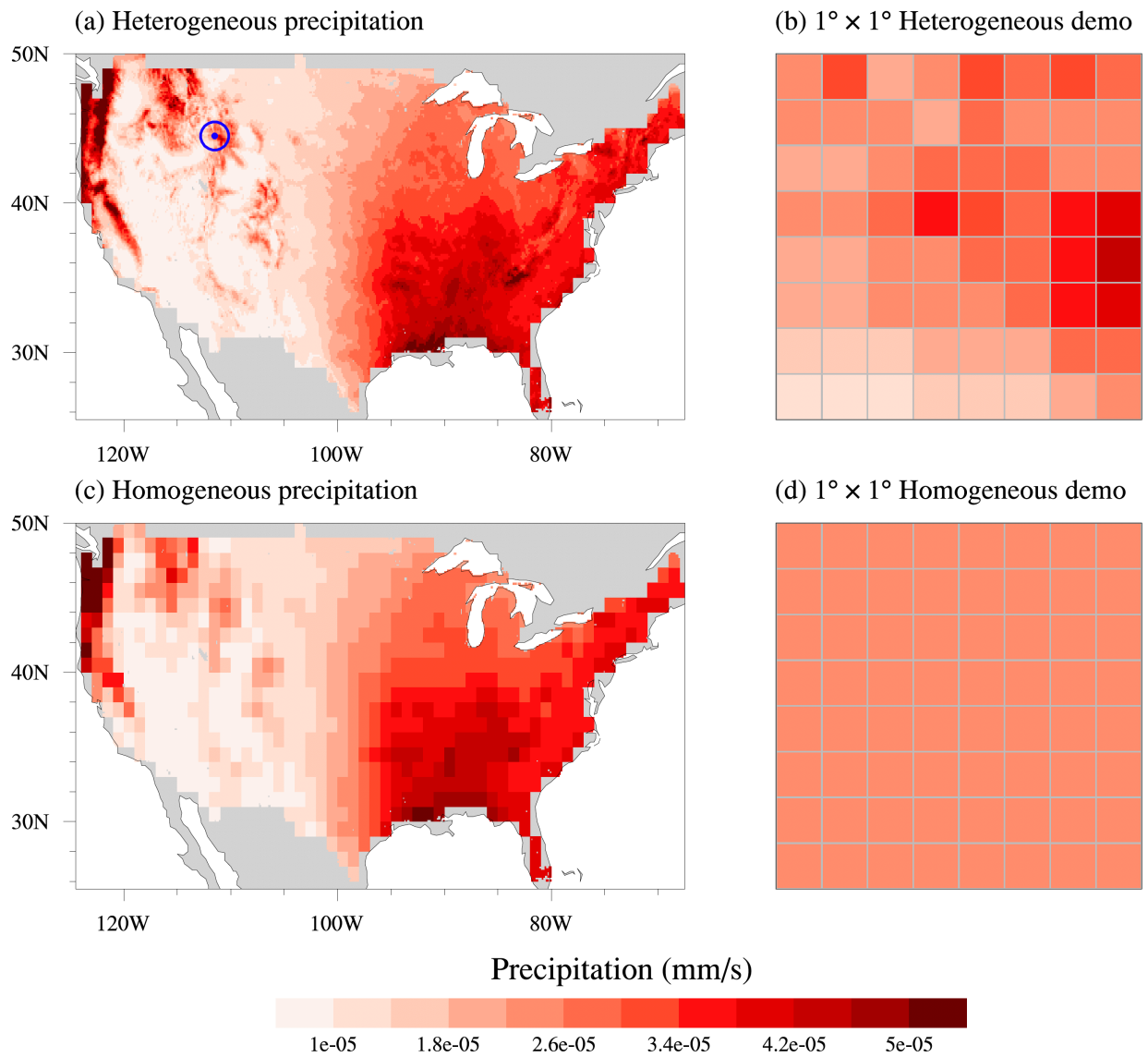
Heterogeneity source	Components	Source data resolution
ATM	Precipitation, air temperature, specific humidity, shortwave radiation, longwave radiation, wind speed, air pressure	$0.125^\circ$ , hourly
SOIL	Soil texture, soil organic matter Soil color	$0.083^\circ$ , static $0.5^\circ$ , static
TOPO	Slope, Standard deviation of elevation, maximum fractional saturated area Fractions of PFTs, wetland, lake, urban characteristics, and glacier	$0.125^\circ$ , static $0.05^\circ$ , static
LULC	LAI for each PFT	$0.05^\circ$ , monthly

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### 160 2.2.2 Heterogeneous and homogeneous inputs

161 We prepared heterogeneous and homogeneous inputs at  $0.125^\circ \times 0.125^\circ$ . The difference between  
 162 the two datasets is whether the input values within each  $1^\circ \times 1^\circ$  region of ELM are spatially  
 163 heterogeneous or homogeneous. The SOIL, TOPO, and LULC were first mapped from their  
 164 original resolutions to  $0.125^\circ \times 0.125^\circ$  resolution, using the Earth System Modeling Framework  
 165 (ESMF) regriding tool. Specifically, the first-order conservative interpolation was used for  
 166 upscaling dataset (e.g., soil texture), while the nearest neighbor interpolation was used for

167 downscaling dataset (e.g., soil color). These  $0.125^\circ$  resolution datasets are used as the  
168 heterogeneous inputs (Figures 1a and 1b). Then, for each dataset, we replaced the heterogeneous  
169 values of the 64  $0.125^\circ \times 0.125^\circ$  grids within each  $1^\circ \times 1^\circ$  region by the mean of the 64 grids (see  
170 Figure 1b vs. 1d). The temporally varying datasets (e.g., hourly ATM and monthly climatology  
171 LAI) were processed at each time interval. As an example, Figure 1 compares the annual  
172 climatology of the heterogeneous and homogeneous precipitation.



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174 Figure 1. Annual climatology of (a) heterogeneous and (c) homogeneous precipitation over  
 175 CONUS. The corresponding (b) heterogeneous and (d) homogeneous precipitation over a  $1^\circ \times 1^\circ$   
 176 region (latitude:  $37^\circ \text{ N} \sim 38^\circ \text{ N}$ , longitude:  $111^\circ \text{ W} \sim 110^\circ \text{ W}$ , the blue marker in (a)) is also shown.  
 177

### 178 **2.3 Experimental design and analysis**

179 We conducted two sets of ELM experiments over CONUS. The first set contains 16 experiments  
 180 with different combinations of heterogeneous and homogeneous inputs from the four heterogeneity  
 181 sources (Table 2). These experiments were used to quantify the influence of different heterogeneity  
 182 sources on the ELM simulations. The second set of 13 experiments were further conducted to  
 183 analyze the impact of heterogeneity from individual components of three heterogeneity sources  
 184 (Table 3). As LULC has no explicit individual component, we only analyzed the components of  
 185 ATM with seven experiments, SOIL with three experiments, and TOPO with three experiments.  
 186 Each experiment only contains one heterogeneous input while other components are homogeneous.  
 187 Both the first and second set of experiments were configured at  $0.125^\circ \times 0.125^\circ$  spatial resolution.  
 188 The 40-year NLDAS-2 forcing from 1980–2019 was cycled twice to drive the ELM run for 80  
 189 years. The first 50-year run was used as model spin-up, and the last 30-year simulation  
 190 (corresponding to atmospheric forcing from 1990–2019) was used for further analysis.

191

192 Table 2. The first set of 16 experiments with inputs from ATM, SOIL, LULC, and TOPO.  
 193 (0 and 1 denote homogeneous and heterogeneous input from the four heterogeneity sources,  
 194 respectively)

No.	Abbr.	ATM	SOIL	LULC	TOPO
EXP1	A0S0L0T0	0	0	0	0
EXP2	A0S0L0T1	0	0	0	1
EXP3	A0S0L1T0	0	0	1	0
EXP4	A0S0L1T1	0	0	1	1
EXP5	A0S1L0T0	0	1	0	0

EXP6	A0S1L0T1	0	1	0	1
EXP7	A0S1L1T0	0	1	1	0
EXP8	A0S1L1T1	0	1	1	1
EXP9	A1S0L0T0	1	0	0	0
EXP10	A1S0L0T1	1	0	0	1
EXP11	A1S0L1T0	1	0	1	0
EXP12	A1S0L1T1	1	0	1	1
EXP13	A1S1L0T0	1	1	0	0
EXP14	A1S1L0T1	1	1	0	1
EXP15	A1S1L1T0	1	1	1	0
EXP16	A1S1L1T1	1	1	1	1

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196 Table 3. The second set of 13 experiments with inputs from each component of the heterogeneity

197

sources.

No.	Sole heterogeneity input
<b>ATM</b>	
ATM1	Precipitation
ATM2	Air temperature
ATM3	Specific humidity
ATM4	Shortwave radiation
ATM5	Longwave radiation
ATM6	Wind speed
ATM7	Air pressure
<b>SOIL</b>	
SOIL1	Soil texture of sand, silt, and clay
SOIL2	Soil organic matter
SOIL3	Soil color
<b>TOPO</b>	
TOPO1	Fmax
TOPO2	Standard deviation of elevation
TOPO3	Slope

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199 Our analysis focused on water partitioning, energy partitioning, and related flux variables. The

200 water partitioning is quantified as the ratio between evapotranspiration (ET) and precipitation (P),

201 i.e., ET/P, and the ratio between runoff (R) and precipitation (P), i.e., R/P. The energy partitioning

202 is quantified using the evaporative fraction (EF), which equals the ratio between latent heat (LH)

203 and the sum of latent heat and sensible heat (SH), i.e.,  $EF = \frac{LH}{LH+SH} * 100 (\%)$ . First, the 30-year



204 monthly, seasonal, and annual climatological means were calculated for each experiment at  
205  $0.125^\circ \times 0.125^\circ$  resolution for the five variables of interest (i.e., P, ET, R, LH, and SH). Second, the  
206 water and energy partitioning variables (i.e., ET/P, R/P, EF) were computed at  $0.125^\circ \times 0.125^\circ$   
207 resolution. Third, the standard deviations (SDs) of these variables' climatological mean were  
208 calculated for each  $1^\circ \times 1^\circ$  region from its embedded 64  $0.125^\circ \times 0.125^\circ$  grids. These  $1^\circ \times 1^\circ$   
209 resolution SDs of the first and second set of experiments were used in following analysis.  
210 For the first set of 16 experiments, we utilized the Sobol' sensitivity analysis to quantify the relative  
211 importance of the four heterogeneity sources on water and energy simulations. Detail of Sobol'  
212 sensitivity analysis is described in section 2.4.  
213 The Sobol' method was not used for the second set of 13 experiments because a comprehensive  
214 Sobol' analysis needs  $2^{13}$  experiments, which is computationally infeasible. Instead, the calculated  
215 SD of each experiment is used to quantify the impact of heterogeneity of each component, as each  
216 experiment only contains one heterogeneous input. Therefore, we compared the SDs between each  
217 experiment to determine the relative importance of each component with heterogeneous input  
218 (without considering interactions between different components).

219

## 220 **2.4 The Sobol' sensitivity indices**

221 The Sobol' sensitivity analysis (Sobol', 1993) was applied to quantify the sensitivity of spatial  
222 variation (i.e., SD) of water and energy partitioning to the four heterogeneity sources based on the  
223 first set of 16 experiments. Here, Sobol' first-order sensitivity index measures the direct  
224 contribution of a single heterogeneity source to the target variable's spatial variability (e.g., EF's  
225 SD). Sobol' higher-order (i.e., second or higher order) sensitivity indices quantify the contribution  
226 by the interactions between a given heterogeneity source with other heterogeneity sources. The

227 sum of all higher-order indices quantifies the overall interaction effects. Sobol' total sensitivity  
 228 index measures the total contribution of a given heterogeneity source, which considers both the  
 229 first-order and the interaction effects (Zhang et al., 2015; Saltelli et al., 2010). Specifically, the  
 230 Sobol' total sensitivity index ( $ST_{X_i}$ ) and the first-order sensitivity index ( $S_{X_i}$ ) are given as (Saltelli  
 231 et al., 2010),

$$232 \quad ST_{X_i} = \frac{E_{X_{\sim i}}(V_{X_i}(Y|X_{\sim i}))}{V(Y)} \quad (1)$$

$$233 \quad S_{X_i} = \frac{V_{X_i}(E_{X_{\sim i}}(Y|X_i))}{V(Y)} \quad (2)$$

234 where  $X_i$  is the  $i$ -th heterogeneity source (e.g., ATM, SOIL, LULC, and TOPO);  $X_{\sim i}$  denotes the  
 235 other heterogeneity sources except  $X_i$ ;  $Y$  is the SD of a given simulated variable for a given  
 236 experiment, and  $V(Y)$  is the total variance of the given variable's SDs across all 16 experiments.

237 Figure 2 illustrates the calculation of Sobol' total and first-order sensitivity indices for LULC (i.e.,  
 238  $X_i = LULC$ ) as follows:

239 (1) For the calculation of  $ST_{X_i}$ : First, following Zheng et al. (2019), the SDs of the 16 experiments  
 240 are reformed into 8 subgroups based on experiments with different combinations of  $X_{\sim i}$ .  
 241 Second, the variance of SD for each subgroup is computed. Third, the mean of SD variances  
 242 across 8 subgroups is computed. Fourth,  $ST_{X_i}$  is calculated using equation (1).

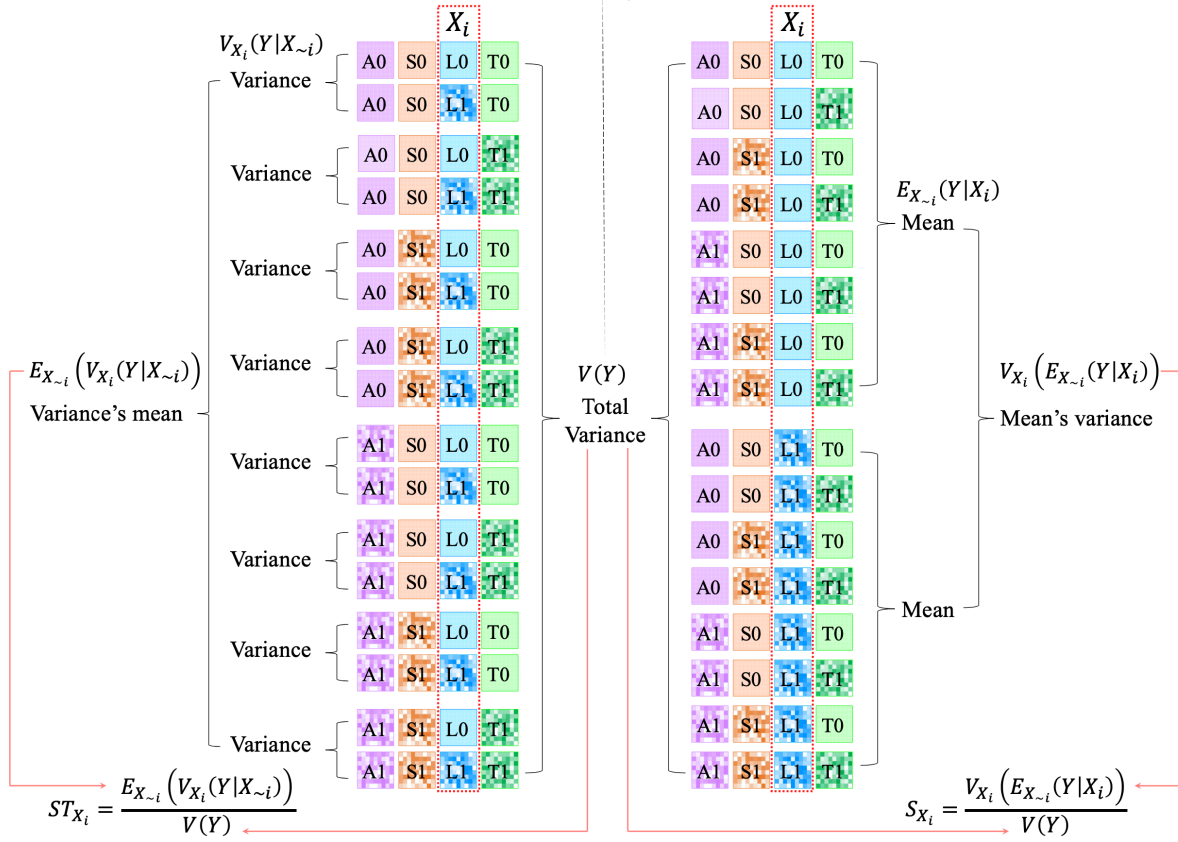
243 (2) For the calculation of  $S_{X_i}$ : First, the SDs of the 16 experiments are reformed into 2 subgroups  
 244 based on the experiments either with heterogeneous or homogeneous  $X_i$ . Second, the mean of  
 245 SDs for each subgroup is computed. Third, the variance of mean SD across 2 subgroups is  
 246 calculated. Fourth,  $S_{X_i}$  is computed using equation (2).

247 The Sobol' sensitivity indices for ATM, TOPO, and SOIL can be computed similarly.

Sobol' total sensitivity index

$Y \rightarrow SD, X_i \rightarrow LULC$

Sobol' first-order sensitivity index



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Figure 2. Schematic flowchart for the calculation of Sobol' total and first-order indices for LULC (i.e.,  $X_i = LULC$ ). The notation (e.g., A0, S0, L0, T0) in each box corresponds to the experiment abbreviation listed in Table 2. A box with (without) mosaic represents heterogeneous (homogeneous) input. The Sobol' total sensitivity index is computed by dividing the 16 experiments into 8 subgroups, such that in each subgroup ATM, SOIL and TOP are fixed except for LULC. The Sobol' first-order sensitivity index is computed by dividing the 16 experiments into 2 subgroups, such that in each subgroup LULC is fixed.

The interaction effect index,  $SI_{X_i}$ , can be computed as,

$$SI_{X_i} = ST_{X_i} - S_{X_i} \quad (3)$$

258 The corresponding fraction of first-order index ( $f_{S_{X_i}}$ ) and interaction effect index ( $f_{SI_{X_i}}$ )  
259 contributing to the total sensitivity index for  $X_i$  can be given as,

$$260 \quad f_{S_{X_i}} = S_{X_i} / ST_{X_i} \times 100 \quad (4)$$

$$261 \quad f_{SI_{X_i}} = 100 - f_{S_{X_i}} \quad (5)$$

262 A more detailed demonstration for the calculation of Sobol' total sensitivity index, first-order  
263 sensitivity index, and the interaction effect index is presented in Appendix A. In this paper, the  
264 Sobol' total sensitivity index is mainly contributed by Sobol' first-order sensitivity index (see  
265 details in section 3.1). Therefore, to make this paper concise, our analysis is based chiefly on Sobol'  
266 total sensitivity index if not explicitly pointed out otherwise.

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## 268 **2.5 ERA5-Land reanalysis dataset**

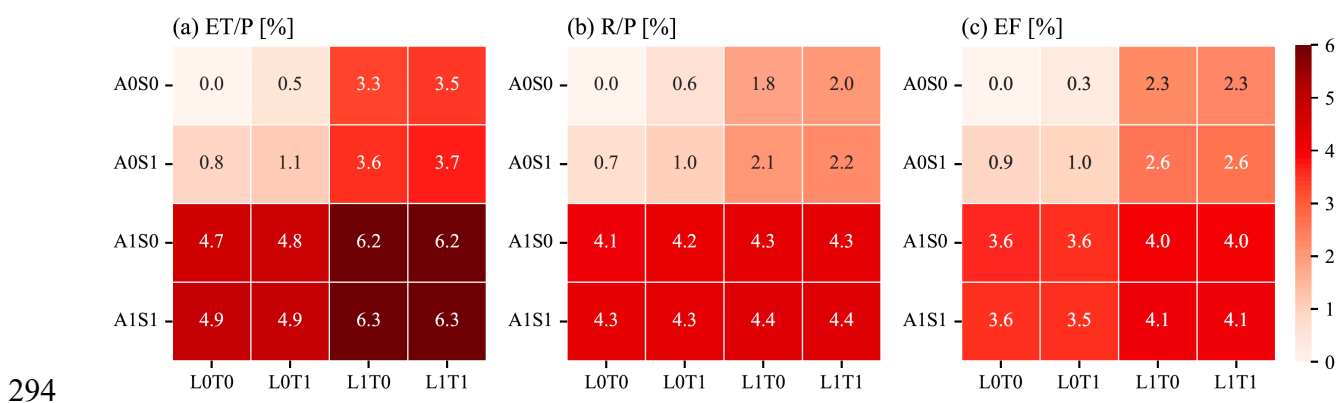
269 We further compared the first set of experiments with ERA5-land reanalysis (the land component  
270 of the fifth generation of European Centre of Medium-range Weather Forecast reanalysis) (Muñoz-  
271 Sabater et al., 2021) to demonstrate the added value in ELM simulations with consideration of  
272 heterogeneity sources. ERA5-Land provides a consistent view of terrestrial water and energy  
273 cycles at high spatial and temporal resolutions. The monthly ERA5-Land data at  $0.1^\circ \times 0.1^\circ$   
274 resolution was used in this study. First, the monthly data was regridded using the ESMF regridding  
275 tool via the first-order conservative interpolation to  $0.125^\circ \times 0.125^\circ$  resolution, which is consistent  
276 with the resolution of our sensitivity experiments. Second, the annual and seasonal climatological  
277 means for related variables (e.g., ET, R, SH) were computed. Third, SD for each variable was  
278 calculated within each  $1^\circ \times 1^\circ$  region for further comparisons with the ELM simulations.

279

280 **3. Results**

281 **3.1. CONUS overall heterogeneity sensitivities**

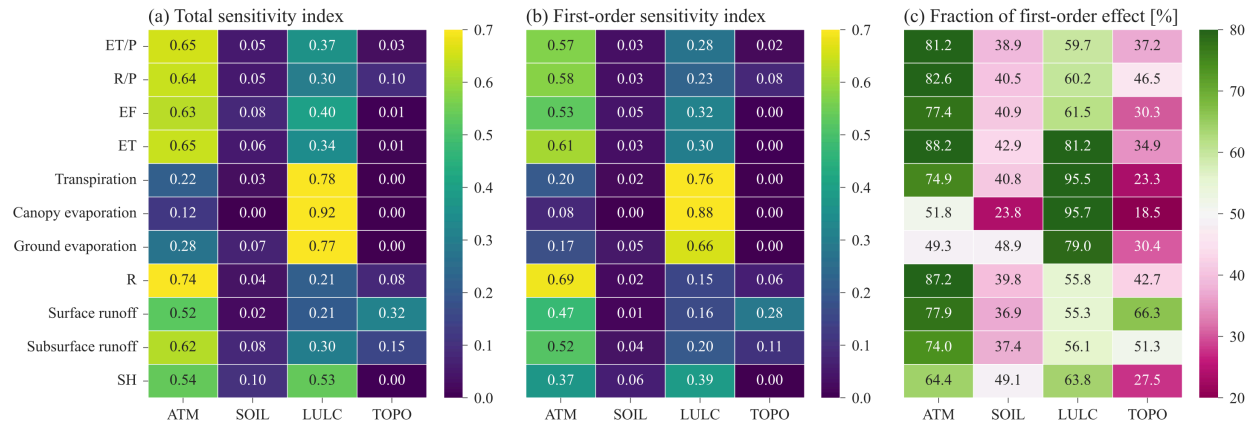
282 The inclusion of more heterogeneity sources leads to larger spatial variability in the simulated  
 283 ET/P, R/P, and EF (Figure 3). For example, comparing experiment A0S0L0T0 with A1S0L0T0  
 284 that includes the ATM heterogeneity, the CONUS averaged SD for ET/P increases from 0 to 4.7%  
 285 (Figure 3a). By further comparing experiments in the first and third rows with the second and  
 286 fourth rows, ATM always increases the spatial variability of water and energy partitioning.  
 287 Similarly, LULC heterogeneity also shows large impacts on the spatial variability for the  
 288 partitioning variables as indicated by comparing experiments in the first and third columns with  
 289 the second and fourth columns. However, heterogeneity in SOIL and TOPO show negligible  
 290 impact. The effects of the heterogeneity sources on the spatial variability of water and energy  
 291 partitioning are mainly located in western and central CONUS (Figure S1), which is consistent  
 292 with the spatial variability of the heterogeneity inputs, for variables such as precipitation, air  
 293 temperature, and longwave radiation (Figure S2).



294 Figure 3. CONUS averaged SD of the annual climatology of (a) ET/P, (b) R/P, and (c) EF.

295 Combining the X-axis label for LULC and TOPO and the Y-axis label for ATM and SOIL  
 296 indicates the names of the experiments listed in Table 2, highlighting the use of heterogeneous  
 297 (1) and homogeneous (0) inputs for each heterogeneity source.

299 ATM, with the largest Sobol' total sensitivity index, is the most important heterogeneity source to  
300 determine the spatial variability of water and energy partitioning (ET/P, R/P, EF in Figure 4a).  
301 LULC is the second most important heterogeneity source (Figure 4a). Even though ATM  
302 dominates the spatial heterogeneity of total ET, LULC is the main contributor to the spatial  
303 variability of the ET components of transpiration, canopy evaporation, and ground evaporation.  
304 The first-order sensitivity indices show similar patterns as the total sensitivity indices (Figure 4b  
305 vs. Figure 4a). For the ATM and LULC, their first-order sensitivity indices contribute more than  
306 60% of the total sensitivity indices in determining the spatial variability of water and energy  
307 partitioning (ET/P, R/P, EF in Figure 4c). Therefore, the total heterogeneity effects of ATM or  
308 LULC are mainly due to their own heterogeneity rather than their interactions with other  
309 heterogeneity sources. The small proportion of the rest of the total heterogeneity effects of ATM  
310 and LULC is contributed by their interactions with other heterogeneity sources (Figure S3b).  
311 The heterogeneity of SOIL and TOPO marginally contributes to the spatial variability of water  
312 and energy partitioning (Figure 4a). Their effects contributed from their own heterogeneity and  
313 their interactions with other heterogeneity sources are relatively small (Figures 4b and S3a). TOPO  
314 shows larger impacts on the spatial variabilities of the runoff components than the total runoff  
315 (Figure 4a). TOPO's impact on the total runoff is mainly due to its interaction effects with other  
316 heterogeneity sources, but its impacts on surface and subsurface runoff are primarily contributed  
317 by its own heterogeneity (Figure 4c).  
318 Generally, high values of total sensitivity indices are mostly contributed by the first-order  
319 sensitivity index (Figures 4a, 4b, and Figure S5). Since our main goal is to analyze the major  
320 heterogeneity sources with a large Sobol' total sensitivity index, the results presented in the  
321 subsequent sections are based chiefly on Sobol' total sensitivity index.



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323 Figure 4. CONUS averaged (a) Sobol' total sensitivity index, (b) Sobol' first-order sensitivity  
 324 index, and (c) the fraction of first-order effect for the sensitivity of spatial variability of different  
 325 variables (rows) to the four heterogeneity sources (columns).

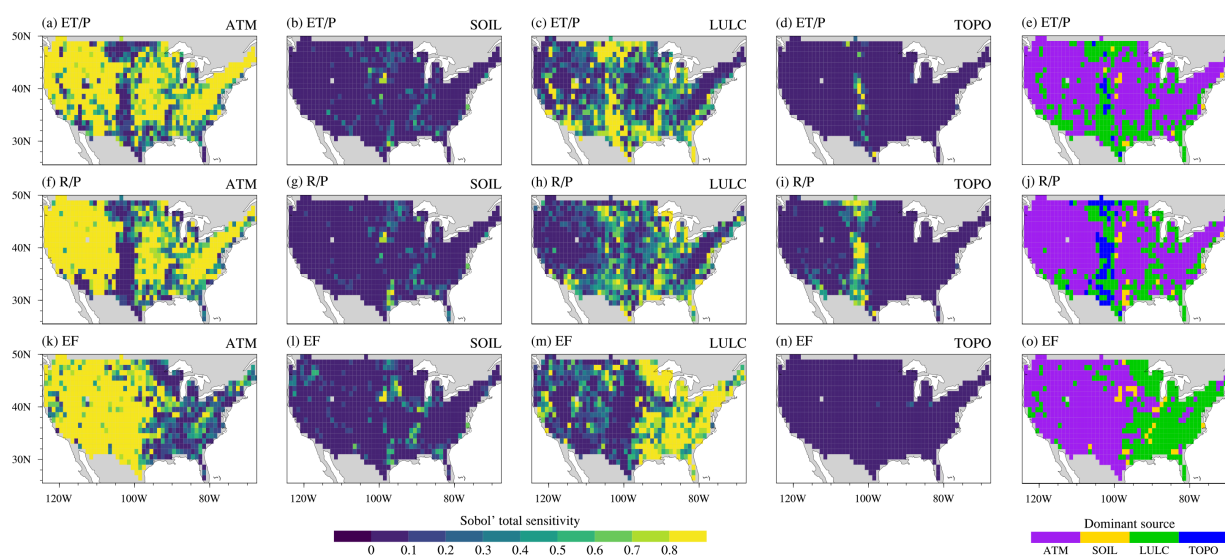
326

### 327 3.2 Spatial patterns of heterogeneity sensitivities

328

329 The sensitivity of the four heterogeneity sources shows different spatial patterns over CONUS  
 330 (Figure 5). The water partitioning components, ET/P and R/P, exhibit similar spatial patterns of  
 331 Sobol' sensitivity index for any given heterogeneity source (Figures 5a-d, 4f-i). ATM shows high  
 332 Sobol' sensitivity index over most CONUS regions for water and energy partitioning. It dominates  
 333 the spatial variability of ET/P and R/P over eastern and western CONUS but not central CONUS  
 334 (Figures 5e and 5j). For the spatial variability of EF, ATM mostly shows dominant effects over  
 335 central and western CONUS (Figures 5o). LULC is the second most dominant heterogeneity  
 336 source and dominates most regions over eastern CONUS, although LULC also dominates smaller  
 337 regions for the spatial variability of ET/P and R/P over central and southeastern CONUS (Figures  
 338 5e and 5j). Overall, ATM Sobol' total sensitivity index has opposite spatial patterns compared to  
 339 LULC Sobol' total sensitivity index (Figure B1 in Appendix B). Therefore, ATM and LULC show  
 340 complementary contributions to the spatial variability of water and energy partitioning across  
 CONUS. Although TOPO overall has low Sobol' index, it dominates the spatial variability of R/P

341 over central CONUS (Figure 5j). SOIL has negligible impacts over most regions of CONUS for  
 342 the spatial variability of both water and energy partitioning. The spatial distributions of Sobol'  
 343 first-order sensitivity indices for the four heterogeneity sources are similar to the Sobol' total  
 344 sensitivity indices (Figure 5 vs. Figure S4). First-order sensitivity indices contribute dominantly  
 345 to the total sensitivity indices (Figure S5). Therefore, most of the heterogeneity effects on water  
 346 and energy partitioning by each heterogeneity source come from its own heterogeneity, with small  
 347 proportions from its interaction effects with other heterogeneity sources.



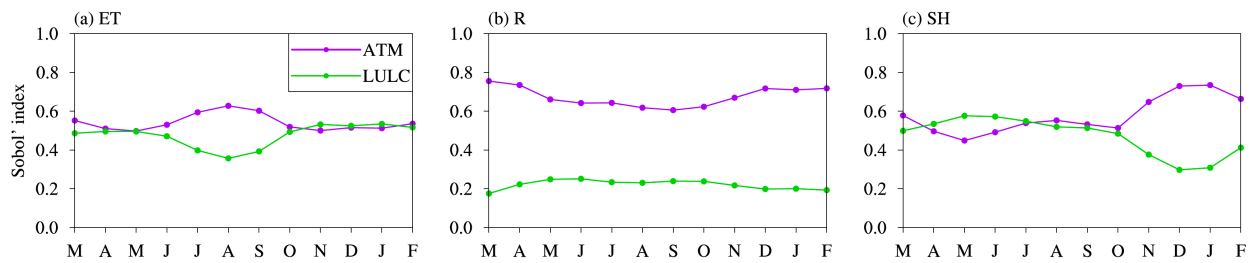
348  
 349 Figure 5. Spatial patterns of Sobol' total sensitivity index for the four heterogeneity sources  
 350 (column 1-4) and the corresponding dominant sources (column 5) for the spatial variability of  
 351 water (ET/P and R/P) and energy (EF) partitioning.

### 353 3.3 Seasonal variation of heterogeneity sensitivities

354 The impacts of ATM and LULC on the spatial variability of water and energy fluxes show more  
 355 seasonal variations than the impacts of SOIL and TOPO (Figure 6, SOIL and TOPO are not shown  
 356 here). This is because ATM and LULC consist of time-varying inputs to the ELM simulations, but



357 SOIL and TOPO are time-invariant inputs. Even though the spatial distribution of LULC is  
 358 temporally static, the monthly variations in LAI and SAI of different land cover types could affect  
 359 the seasonal variation of sensitivity. The heterogeneity impacts of ATM and LULC on the spatial  
 360 variability of water and energy fluxes show complementary seasonal variations. The effect of  
 361 ATM on the ET spatial variability is larger in July–September than in other months (Figure 6a),  
 362 while LULC shows smaller Sobol' index in July–September. The sensitivity of transpiration and  
 363 canopy evaporation shows the same seasonal variations (Figures C1d~f in Appendix C). The  
 364 spatial variability of R is more sensitive to ATM in the cold season (December–April, Figure 6b),  
 365 especially for its component of surface runoff (Figure C1g). The sensitivity of SH spatial  
 366 variability to ATM is larger in the non-growing season (i.e., November–March) than in the  
 367 growing season (i.e., April–October), with the LULC Sobol' index showing opposite seasonal  
 368 variations (Figure 6c).



369  
 370 Figure 6. Monthly variations of CONUS averaged ATM and LULC Sobol' index for (a) ET, (b)  
 371 R, and (c) SH.

372  
 373 The spatial patterns of dominant regions by the four heterogeneity sources vary over different  
 374 seasons. Compared with spring and winter, ATM dominates the ET spatial variability in more  
 375 regions than in summer and fall when ATM is more dominant over eastern CONUS (Table 5 and  
 376 Figures S6a~d). LULC shows opposite seasonal spatial patterns with more dominant regions in

377 eastern CONUS over spring and winter. As for the R spatial variability, TOPO shows large spatial  
378 variation of its dominant regions over different seasons (Figures S6f~i). Besides its dominant  
379 contribution in central CONUS over all seasons, TOPO also dominates the R spatial variability in  
380 parts of eastern US in the summer and autumn (Figures S6g~h). For the EF spatial variability,  
381 ATM has more contributions in the fall and winter but smaller contributions in spring and summer  
382 than LULC (Table 5). LULC shows more dominant regions over eastern CONUS, especially in  
383 spring and summer (Figures S6k~i). To understand the seasonal variations of dominant  
384 heterogeneity sources, the seasonal variations of Sobol' total sensitivity index and induced R's SD  
385 are demonstrated at one gridcell over eastern US (Figure S7). Compared with other heterogeneity  
386 sources, ATM induced R's SD shows an apparent seasonal variation, with high values in spring  
387 and winter but small values in summer and fall (Figure S7b). Therefore, ATM is the dominant  
388 heterogeneity source in spring and winter. Even though TOPO and SOIL induced R's SDs show  
389 slight seasonal variations (Figure S7), they dominate R's spatial variability in summer and fall,  
390 respectively.

391 Table 5 Grid percentage of the dominant heterogeneity source in determining the spatial  
392 variability of ET, R, and SH for four seasons and annual mean (ANN)

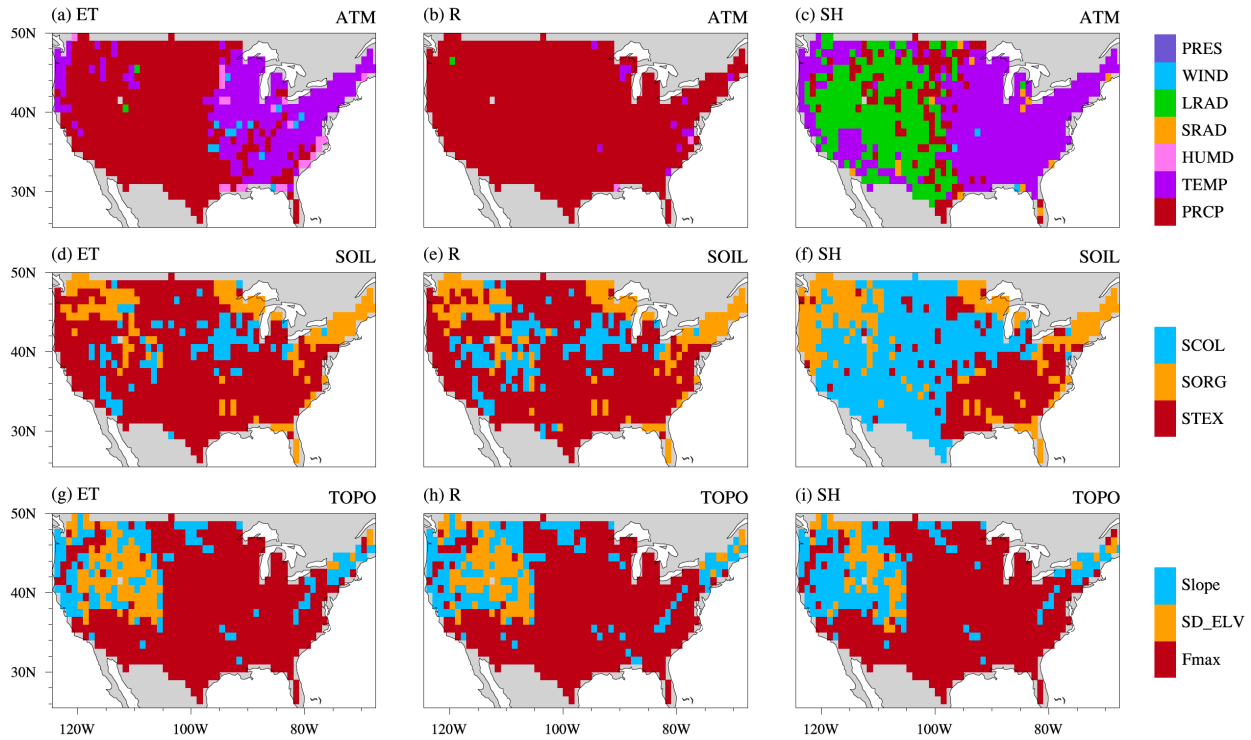
Seasons	ATM	SOIL	LULC	TOPO
<b>ET</b>				
Spring (MAM)	51	4	46	0
Summer (JJA)	63	3	34	0
Fall (SON)	57	2	42	0
Winter (DJF)	49	0	51	0
ANN	66	2	31	0
<b>R</b>				
Spring (MAM)	81	2	13	5
Summer (JJA)	67	4	17	11
Fall (SON)	66	6	18	11
Winter (DJF)	75	2	12	10
ANN	77	1	15	7
<b>SH</b>				
Spring (MAM)	44	5	51	0
Summer (JJA)	45	2	53	0
Fall (SON)	52	5	44	0

Winter (DJF)	69	2	29	0
ANN	49	4	47	0

393

394 **3.4 Effects of ATM heterogeneity components**

395 Based on the second set of 13 experiments, we analyzed the heterogeneity effects by each  
396 component of ATM, SOIL, and TOPO (Figure 7), respectively. Precipitation is the largest ATM  
397 heterogeneity source in determining the spatial variability of water fluxes (Figures 7a~b),  
398 especially over western and central CONUS for ET (Figure 7a) and almost the entire CONUS for  
399 R (Figure 7b). Air temperature dominates the spatial variability of ET in eastern CONUS (Figure  
400 7a). The spatial variability of SH is mainly dominated by the incoming longwave radiation in  
401 western CONUS and by the air temperature in eastern CONUS (Figure 7c). Longwave radiation  
402 provides more energy input and contributes more to the SH spatial variability than shortwave  
403 radiation (Figure 8c). Among the SOIL components, soil texture, which can influence soil moisture  
404 and runoff generation, shows the largest effects on the ET and R spatial variability over most  
405 CONUS regions (Figures 7d, 7e, 8d, and 8e). Soil color, affecting the surface albedo and energy  
406 balance, shows the largest impacts on the SH spatial variability over central CONUS (Figures 7f  
407 and 8f). Fmax is the most essential TOPO component, offering the largest effects on the spatial  
408 variability of ET, R, and SH over most CONUS regions (Figures 7g~i and Figures 8g~i). Fmax  
409 regulates surface runoff generation and infiltration, and therefore influences the soil moisture, ET,  
410 and SH. SD\_ELV and slope can affect surface water and snow cover fraction, and consequently,  
411 they show the largest impacts over northwestern CONUS regions with mountains and snowpack.

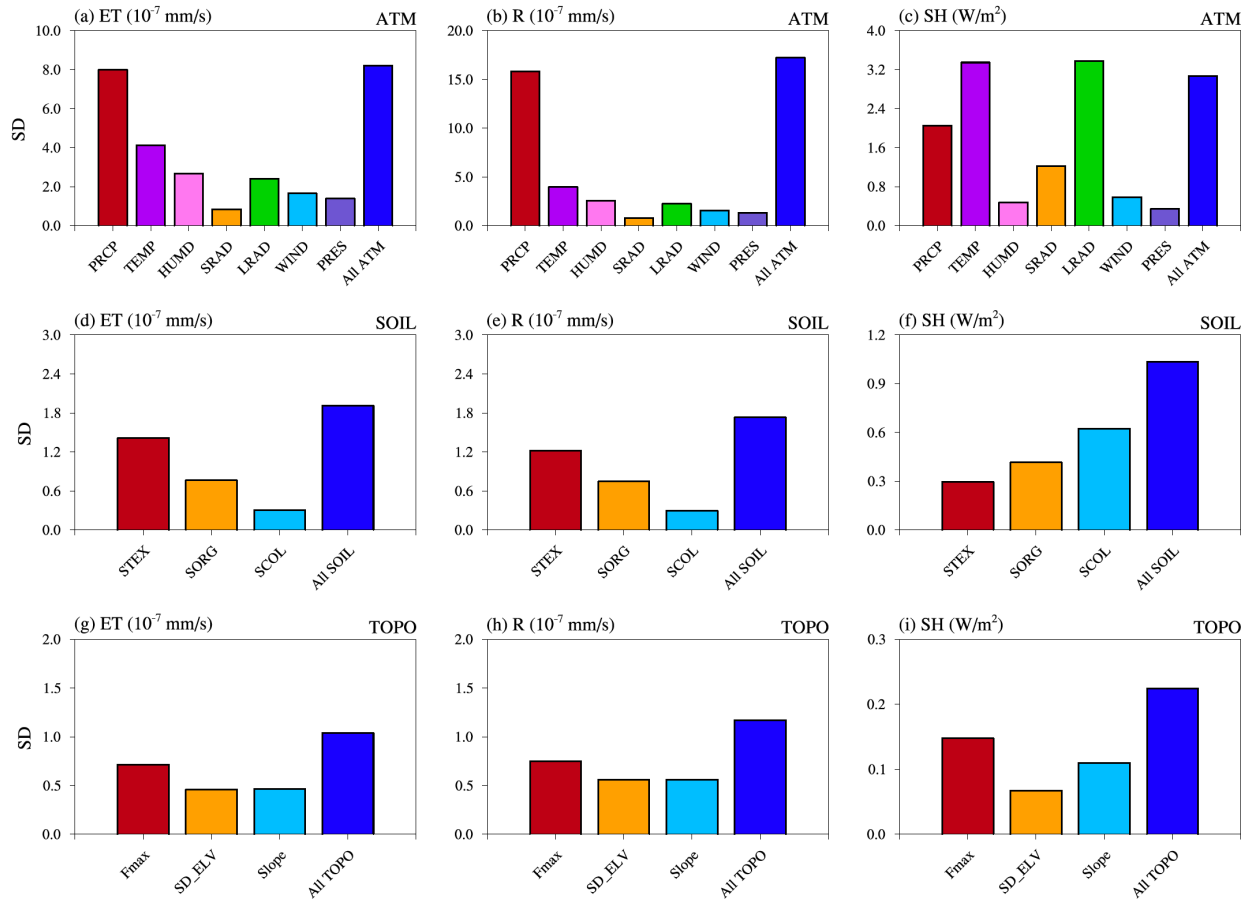


412

413 Figure 7. The largest induced spatial variability for the annual climatological mean of ET (left  
 414 column), R (middle column), and SH (right column) induced by each component of ATM (top  
 415 panel), SOIL (middle panel), and TOPO (bottom panel)

416

417 The spatial variability induced by all components (of ATM, SOIL, or TOPO) is larger than that  
 418 induced by each individual component. However, it is smaller than the sum of the spatial  
 419 variability induced by each component (Figure 8). For example, the CONUS averaged SD for ET  
 420 caused by all SOIL components is  $1.9 (10^{-7} \text{ mm/s})$ , which is smaller than  $2.5 (10^{-7} \text{ mm/s})$ , the sum  
 421 of the SD of ET induced by STEX, SORG, and SCOL (Figure 8d). Therefore, the additional SD  
 422 induced by an additional heterogeneity component decreases, suggesting that the effect of  
 423 heterogeneity on the spatial variability of water and energy fluxes saturates, due to the interaction  
 424 effects between heterogeneity components on related water and energy processes.



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### 3.5 Comparison with ERA5-Land reanalysis

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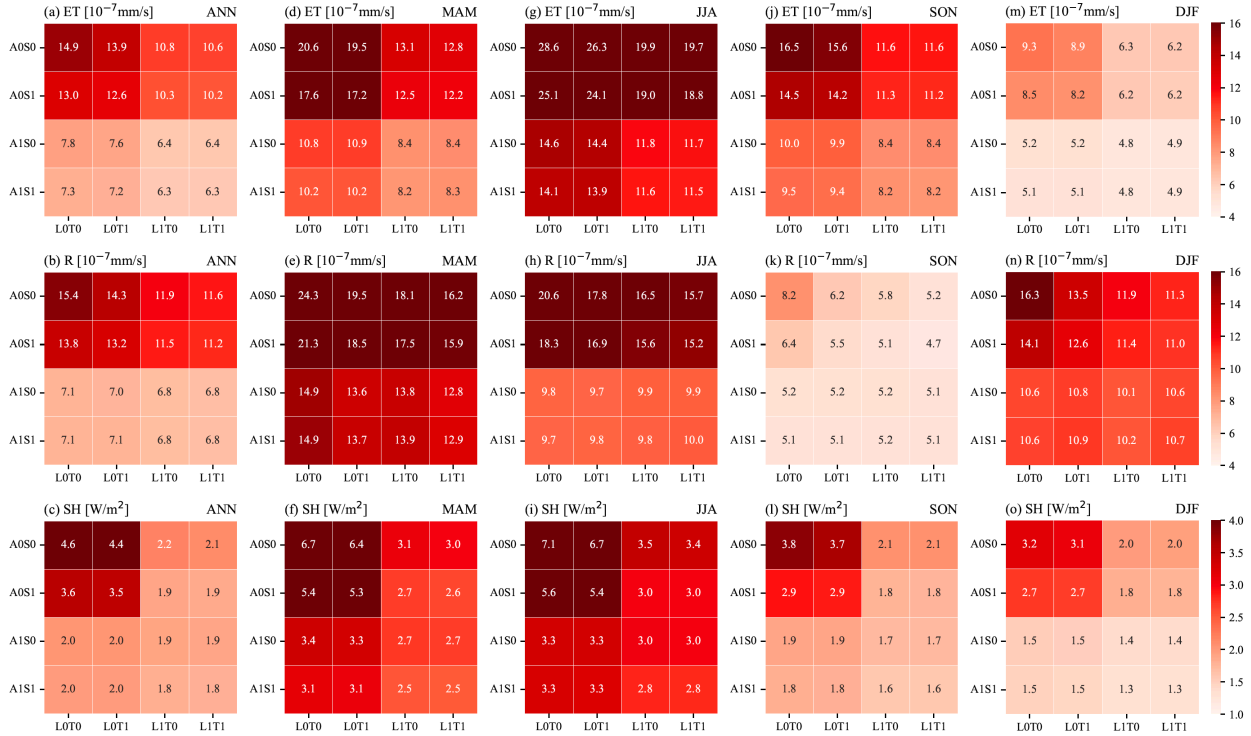
436

Figure 8. CONUS averaged spatial variability for the annual climatological mean of ET (left column), R (middle column), and SH (right column) by each component and all components of ATM (top panel), SOIL (middle panel), and TOPO (bottom panel).

Higher consistency of the spatial variability between the simulations and ERA5-Land reanalysis (i.e., smaller SD difference) is obtained when more sources of heterogeneity are accounted for in the simulations for ET, R, and SH (Figure 9). ATM and LULC dominate the improvements in the spatial variability of model simulations. Generally, ATM heterogeneity leads to more or similar improvements than LULC heterogeneity for ET, R, and SH over all seasons. For example, in Figure 9a, ATM induced larger improvements, as shown by comparing experiments in the first

437 and third rows with the second and fourth rows, than the LULC induced improvements, comparing  
438 experiments in the first and third columns with the second and fourth columns. The SD difference  
439 is usually larger over MAM and JJA than SON and DJF, probably due to the heterogeneity  
440 difference between the NLDAS and ERA5 atmosphere forcing as ATM is the major heterogeneity  
441 contributor.

442 Improvements of the spatial variability of model simulations are primarily distributed over western  
443 and eastern CONUS for ET, R, and SH (e.g., Figures S8 and S9 1<sup>st</sup> column vs. 4<sup>th</sup> column). Overall,  
444 the ELM simulated ET and SH have smaller SDs than those of ERA5\_Land (Figures S9d and S9f).  
445 Meanwhile the simulated R has larger SD especially in the western US than that of ERA5\_Land,  
446 probably mainly due to ATM's heterogeneity effects (Figures S9e vs. S9g). For ET and R, ATM  
447 mainly increases their spatial variability over western and eastern CONUS (Figures S8a vs. S8c,  
448 and S8e vs. S8g), and LULC mostly shows changes over eastern CONUS (Figures S8a vs. S8b,  
449 and S8e vs. S8f). Both ATM and LULC increase SH spatial variability over western and eastern  
450 CONUS (Figure S8i vs. S8j, and S8i vs. S8k).



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#### 4. Discussions

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Figure 9. CONUS averaged absolute difference of SD between 16 ELM experiments and ERA5-Land reanalysis for the annual (1<sup>st</sup> column) and seasonal (2<sup>nd</sup> – 5<sup>th</sup> column) climatological mean of ET (top panel), R (middle panel), and SH (bottom panel).

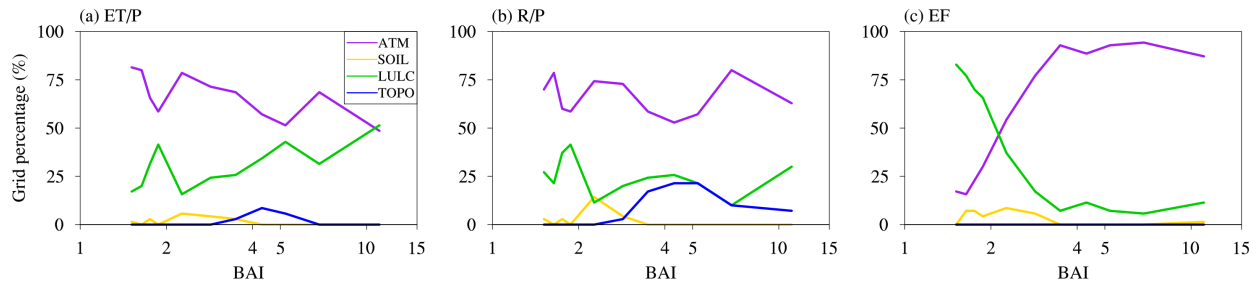
465 climate models is crucial for modeling the water and energy partitioning, especially for the three  
466 major components of precipitation, air temperature, and longwave radiation. Tesfa et al. (2020)  
467 compared several simple approaches to capturing ATM heterogeneity for downscaling the grid  
468 mean precipitation to topography-based subgrids for land surface modeling. Besides ATM, LULC  
469 is the second most crucial heterogeneity source. Notably, anthropogenic land use and land cover  
470 change has been shown to have large impacts on land–atmosphere interaction, land surface  
471 hydrology, and associated extreme events (Findell et al., 2017; Li et al., 2018, 2015; Swann et al.,  
472 2010; Zeng et al., 2017; Yuan et al., 2021; PIELKE et al., 2007). Therefore, the heterogeneity of  
473 LULC should also be well considered in climate modeling.

474

475 ATM and LULC show complementary contributions to the spatial variability of water and energy  
476 partitioning spatially over CONUS and temporally in different seasons. Sobol' sensitivity analysis  
477 is a standardized quantification of the relative importance of different heterogeneity sources. The  
478 sum of the Sobol' indices for the four heterogeneity sources roughly equals one. As the two  
479 dominant heterogeneity sources, ATM Sobol index and LULC Sobol' index dominate the sum of  
480 all Sobol' indices. Hence, they show complementary patterns spatially (Figure B1) and temporally  
481 (Figure 6). In addition, ATM and LULC show complementary contributions across different  
482 climate zones. The Budyko's aridity index (BAI, Budyko 1974), which is the ratio of annual net  
483 radiation to the product of the latent heat of water vaporization and the annual precipitation, was  
484 calculated using the outputs from EXP16. From humid (low BAI) to arid climate (high BAI), a  
485 decreasing fraction of the CONUS region is dominated by ATM in determining the ET/P spatial  
486 variability (Figure 10a). At the same time, LULC shows an increasing contribution to the ET/P  
487 spatial variability with BAI. The spatial variability of energy partitioning exhibits even more



488 complementarity between the ATM and LULC contributions from arid regions to humid regions  
 489 (Figure 10c). In more arid regions limited by water, EF spatial variability is much more dominated  
 490 by heterogeneity of ATM, likely through the heterogeneous precipitation, but in humid regions  
 491 limited by energy, LULC dominates the EF spatial variability through its influence on surface  
 492 albedo and surface roughness.



493  
 494 Figure 10. The grid percentage of dominant heterogeneity sources along with Budyko's aridity  
 495 index. A higher aridity index means more arid.

496  
 497 SOIL and TOPO show relatively small impacts on the spatial variability of water and energy  
 498 partitioning. However, TOPO has a dominant influence on the R/P spatial variability over the  
 499 transitional zone (Figure 10b) of central CONUS located between the arid western CONUS and  
 500 the humid eastern CONUS (Figure 5). TOPO's impact on the total runoff is mainly due to its  
 501 interaction effects with other heterogeneity sources (Figure 4). SOIL shows some dominant effects  
 502 on the spatial variability of water and energy partitioning over a small proportion of humid regions  
 503 (Figure 10). The heterogeneity in SOIL and TOPO was derived from coarse resolution data at  
 504  $0.125^{\circ} \times 0.125^{\circ}$  spatial resolution, which could be a possible reason for the minor SOIL and TOPO  
 505 effects. Singh et al. (2015) found that CLM4.0 did not show much improvement when model  
 506 resolution increased from  $\sim 100$  km to  $\sim 25$  km but improvement was noticeable at finer 1 km

507 resolution. Additionally, exclusion of lateral subsurface flow in ELMv1 could also lead to  
508 underestimation of the contributions from SOIL and TOPO.

509

510 The current study excluded a few land surface processes that have been included in LSMs in the  
511 last decade, limiting our ability to assess the role of land surface heterogeneity in spatiotemporal  
512 variability of energy and water partitioning. For example, the hillslope processes of lateral ridge-  
513 valley flow and the insolation contrasts between sunny and shady slopes are crucial for land surface  
514 modeling (Fan et al., 2019; Taylor et al., 2012; Clark et al., 2015; Scheidegger et al., 2021), but  
515 they are neglected in this study. Sean et al. (2019) incorporated the representative hillslope concept  
516 into the CLM5, and they found that subgrid hillslope process induced large differences in  
517 evapotranspiration between upland and lowland hillslope columns in arid and semiarid regions.  
518 Krakauer et al. (2014) suggested that the magnitude of between-grid groundwater flow becomes  
519 significant over larger regions at higher model resolution. Xie et al. (2020) also demonstrated the  
520 importance of groundwater lateral flow in offsetting depression cones caused by intensive  
521 groundwater pumping. Fang et al. (2017) compared the ACME Land Model (the earlier version of  
522 ELM) and the three-dimensional ParFlow variably saturated flow model (Maxwell et al., 2015),  
523 underscoring ELM limitation in capturing topography's influence on groundwater and runoff.  
524 Additionally, topography also significantly influences insolation, including the shadow effects and  
525 multi-scattering between adjacent terrain. Hao et al. (2021) implemented a sub-grid topographic  
526 parameterization in ELM, which improves the simulated surface energy balance, snow cover, and  
527 surface air temperature over the Tibetan Plateau. The inclusion of plant hydraulics has also shown  
528 essential improvements in water and carbon simulations under drought conditions (Li et al., 2021;  
529 Fang et al., 2021), which should also be considered in future research, especially as vegetation

530 may experience more hydroclimate drought stress in projected future climate conditions (Yuan et  
531 al., 2019; Xu et al., 2019; Li et al., 2020). The subgrid downscaling of atmospheric forcing (Tesfa  
532 et al., 2020), which could further enhance the representation of heterogeneity effects on water and  
533 energy simulations, is also unaccounted for in this study.

534

## 535 **5. Conclusions**

536 This study comprehensively investigated the impacts of different heterogeneity sources (i.e., ATM,  
537 LULC, SOIL, TOPO) on the spatial variability of water and energy partitioning over CONUS.  
538 Two sets of experiments were conducted based on different combinations of spatially  
539 heterogeneous and homogeneous datasets. Based on the first set of 16 experiments, Sobol' total  
540 and first-order sensitivity indices were utilized to identify the relative importance of the four  
541 heterogeneity sources. The second set of 13 experiments were further used to assess the influence  
542 from individual components of ATM, SOIL, and TOPO. Our results show that ATM and LULC  
543 are the two dominant heterogeneity sources in determining the spatial variability of water and  
544 energy partitioning, largely contributed by ATM's or LULC's own heterogeneity and slightly  
545 contributed by their interactions with other heterogeneity sources. Their heterogeneity effects are  
546 spatially complementary across CONUS, and temporally complementary across seasons. The  
547 complementary contributions of ATM and LULC reflect the overall negligible impacts of SOIL  
548 and TOPO, but the complementarity also reflects physically the clear demarcation of climatic  
549 zones across CONUS, featuring the arid, water-limited western CONUS dominantly influenced  
550 by ATM (precipitation in particular) and the humid, energy-limited eastern CONUS dominantly  
551 influenced by LULC. In the transitional climate zone of central CONUS, TOPO shows some  
552 dominant influence on the R/P spatial variability. The overall most essential components for ATM

553 (precipitation, temperature, and longwave radiation), SOIL (soil texture and soil color), and TOPO  
554 (Fmax) were also identified. Comparison with ERA5-Land reanalysis reveals that accounting for  
555 more sources of heterogeneity improved the simulated spatial variability of water and energy  
556 fluxes, although such improvements tend to saturate as more heterogeneous sources were added.  
557 The relative importance of different heterogeneity sources quantified in this study is useful for  
558 prioritizing spatial heterogeneity to be included for improving land surface modeling. We note,  
559 however, that the present assessment is limited by how well the input datasets capture the  
560 spatiotemporal heterogeneity and how well the land surface model represents processes such as  
561 hillslope hydrology and topographic effect on solar radiation that are influenced by land surface  
562 heterogeneity. This motivates the use of more process-rich models such as distributed or three-  
563 dimensional subsurface hydrology models to provide benchmarks of the relative importance of  
564 heterogeneity sources to help prioritize future development of land surface models to improve  
565 modeling of energy and water fluxes.

566

567 **Appendix A: demonstration of Sobol' index calculation**

568 Here we give an example for the calculation of Sobol' total, first-order and interaction effect  
 569 indices,  $ST_{LULC}$ ,  $S_{LULC}$ , and  $SI_{LULC}$  to quantify the sensitivity of EF's spatial variability to LULC  
 570 in a  $1^\circ \times 1^\circ$  region at 39.5N and 107.5W.

571 (1) Calculation of  $ST_{LULC}$  (Table A1): Following Zheng et al. (2019), and based on equation (1)  
 572 and Figure 2, the 16 experiments are grouped into 8 subgroups containing two experiments, where  
 573 the difference between the two experiments in a given subgroup is homogeneous vs. heterogeneous  
 574 LULC. The SDs of the 16-experiments are listed in C1. The variance of each subgroup is computed  
 575 in C2, which represents the influence of LULC heterogeneity. The average impact of LULC  
 576 heterogeneity from the eight subgroups in C3 is computed as the mean of the values in C2. The  
 577 total variance of these 16 SDs in C1 is computed in C4. Finally, the ratio between C3 and C4 is  
 578 calculated as Sobol' total sensitivity index in C5, which quantifies EF spatial variability sensitivity  
 579 to LULC heterogeneity.

580 (2) Calculation of  $S_{LULC}$  and  $SI_{LULC}$ : Similarly, based on the equations (2) and (3) and Figure 2,  
 581 we then compute the Sobol' first-order sensitivity index (Table A2) and the Sobol' interaction effect  
 582 index (Table A3), and their contribution fractions to the total sensitivity index (Table A3).

583 Table A1 Calculation of Sobol' total sensitivity index

Experiments	$Y _{\sim LULC}$	$V_{LULC}(Y _{X_{\sim LULC}})$	$E_{\sim LULC}(V_{LULC}(Y _{X_{\sim LULC}}))$	$V(Y)$	$ST_{LULC}$
C0	C1	C2	C3	C4	C5
A0S0L0T0	0.00				
A0S0L1T0	5.24	6.88			
A0S0L0T1	0.57				
A0S0L1T1	5.58	6.28			
A0S1L0T0	0.32				
A0S1L1T0	5.51	6.75	3.32	26.99	0.12
A0S1L0T1	0.69				
A0S1L1T1	5.84	6.64			
A1S0L0T0	12.88				
A1S0L1T0	12.67	0.01			
A1S0L0T1	12.80	0.00			

A1S0L1T1	12.76	
A1S1L0T0	12.71	0.01
A1S1L1T0	12.51	
A1S1L0T1	12.63	0.00
A1S1L1T1	12.59	

584

585

Table A2 Calculation of Sobol' first-order sensitivity index

Experiments	$Y LULC$	$E_{\sim LULC}(Y X_{LULC})$	$V_{LULC}(E_{\sim LULC}(Y X_{LULC}))$	$V(Y)$	$S_{LULC}$
C0	C1	C2	C3	C4	C5
A0S0L0T0	0.00				
A0S0L0T1	0.57				
A0S1L0T0	0.32				
A0S1L0T1	0.69				
A1S0L0T0	12.88	6.58			
A1S0L0T1	12.80				
A1S1L0T0	12.71				
A1S1L0T1	12.63				
A0S0L1T0	5.24		1.58	26.99	0.058
A0S0L1T1	5.58				
A0S1L1T0	5.51				
A0S1L1T1	5.84	9.09			
A1S0L1T0	12.67				
A1S0L1T1	12.76				
A1S1L1T0	12.51				
A1S1L1T1	12.59				

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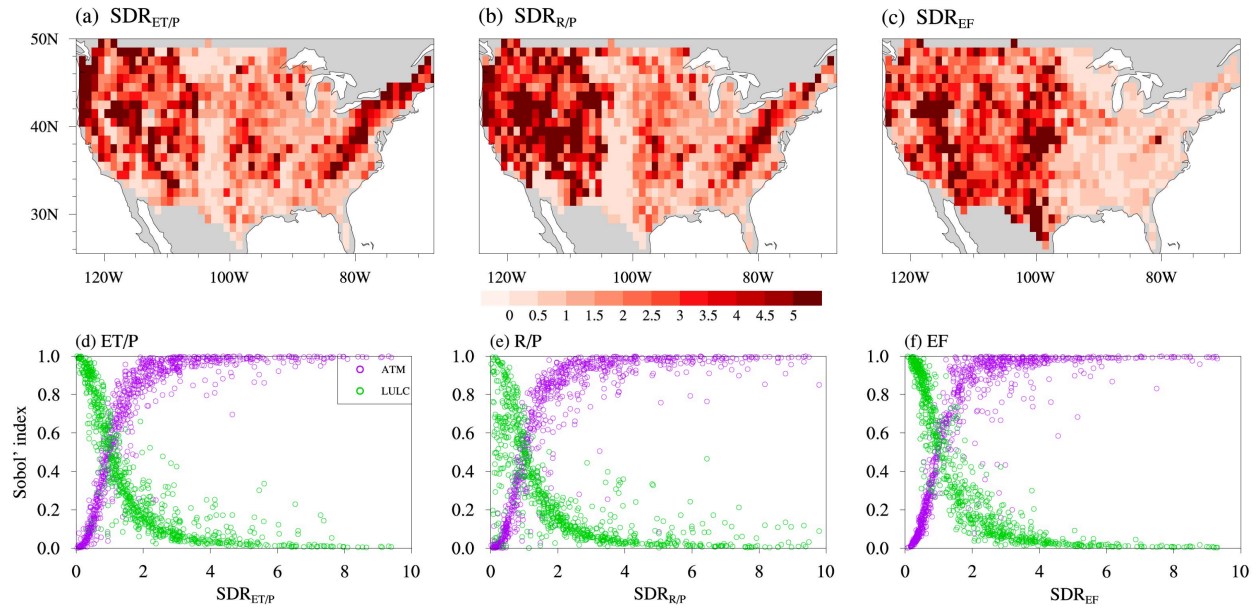
Table A3 Calculation of Sobol' interaction effect index and contributing fractions

	$ST_{LULC}$	$S_{LULC}$	$SI_{LULC}$
Index value	0.12	0.058	0.065
Fraction to total		47.5%	52.5%

588

## 589 **Appendix B: Spatial patterns of Sobol' total sensitivity index vs. SD ratio**

590 To further understand the spatial patterns of the Sobol' total sensitivity index for the two most  
591 dominant heterogeneity sources of ATM and LULC (Figure 5), we further analyzed EXP9  
592 (A1S0L0T0) and EXP3 (A0S0L1T0) listed in Table 2. EXP9 and EXP3 only include  
593 heterogeneous inputs from ATM and LULC, respectively. Let us consider ET/P as the quantity of  
594 interest for the following discussion. First, the SD of ET/P is computed from the annual  
595 climatology (section 2.3). Next, the SD ratio of ET/P, denoted as  $SDR_{ET/P}$ , is computed as the  
596 ratio between the SD of ET/P in EXP9 and EXP3.  $SDR_{ET/P}$  represents the relative spatial  
597 variability induced by ATM compared to LULC (Figure B1a). The spatial pattern of the ATM  
598 Sobol' total sensitivity index for the ET/P spatial variability shows a positive relationship with the  
599 spatial pattern of  $SDR_{ET/P}$  (purple circles in Figure B1d, corresponding to Figure 5a vs. Figure  
600 B1a). Therefore, a higher value of  $SDR_{ET/P}$  indicates that relative to LULC, ATM induces larger  
601 ET/P spatial variability, and hence has a higher ATM Sobol' total sensitivity index. Similarly, a  
602 lower value of  $SDR_{ET/P}$  indicates LULC induces larger ET/P spatial variability than ATM, and  
603 hence has a higher LULC Sobol' total sensitivity index (green circles in Figure B1d). Similarly,  
604  $SDR_{R/P}$  and  $SDR_{EF}$  were calculated for R/P and EF, and they also show a positive (negative)  
605 relationship with the corresponding ATM (LULC) Sobol' total sensitivity index (Figures B1b, B1c,  
606 B1e, and B1f). We can also see that the ATM Sobol' total sensitivity index has opposite spatial  
607 patterns compared to the LULC Sobol' total sensitivity index. Therefore, ATM and LULC show  
608 complementary contributions to the spatial variability of water and energy partitioning across  
609 CONUS.



610

611 Figure B1. Spatial patterns of SD ratios (top panel) and their spatial relationship with the ATM  
 612 and LULC Sobol' total sensitivity index (bottom panel) for ET/P, R/P and EF, respectively. The  
 613 y-axis values correspond to the spatial patterns of the Sobol' total sensitivity index for ATM (purple)  
 614 and LULC (green) in Figure 5 (i.e., each circle corresponds to each  $1^\circ \times 1^\circ$  region).

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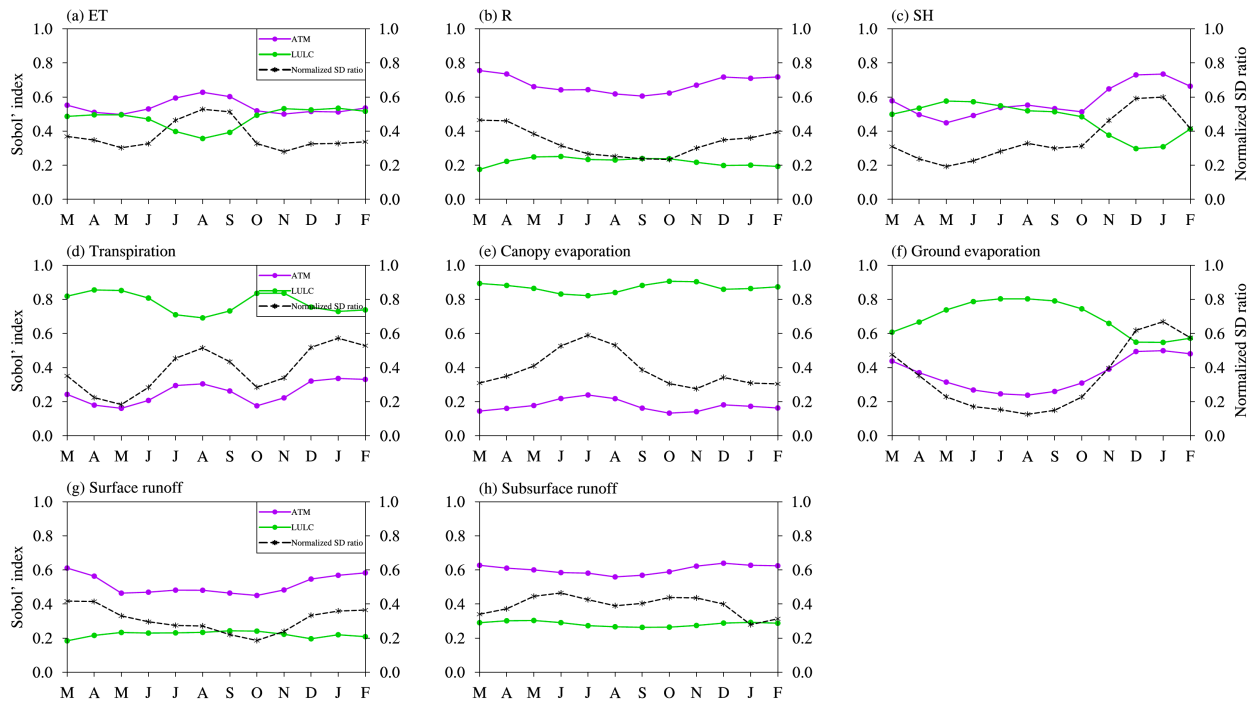
616



617 **Appendix C: Seasonal variations of Sobol' total sensitivity index vs. normalized SD ratio**

618 To further explain the seasonal variations of the Sobol' total sensitivity index for ATM and LULC,  
619 the SD of ET for each month was calculated as an example from monthly mean climatology. The  
620 SD ratio for each month was computed as the ratio between the SD of ET in EXP9 and EXP3. For  
621 each  $1^\circ \times 1^\circ$  region, the 12 monthly SD ratios were normalized to [0, 1] using minimum and  
622 maximum values. Finally, the CONUS average of the normalized SD ratios was computed for each  
623 month, denoted as  $NSDR_{ET}$ . A higher value of  $NSDR_{ET}$  denotes ATM induces more ET spatial  
624 variability than LULC. Therefore,  $NSDR_{ET}$  shows similar seasonal variations with the ATM  
625 Sobol' total sensitivity index for ET spatial variability (black curve vs. purple curve in Figure C1a),  
626 but opposite seasonal variations with the LULC Sobol' total sensitivity index (black curve vs. green  
627 curve in Figure C1a). Similarly, normalized SD ratios were calculated for R, SH, ET components  
628 and R components, and they also show a similar (opposite) seasonal variation with the  
629 corresponding seasonal ATM (LULC) Sobol' total sensitivity index (Figures C1).

630



631

632 Figure C1. Monthly variations of CONUS averaged ATM and LULC Sobol' total sensitivity index

633 to ATM and normalized SD ratio for (a) ET, (b) R, and (c) SH, (d) Transpiration, (e) Canopy

634 evaporation, (f) Ground evaporation, (g) Surface runoff, and (h) Subsurface runoff, respectively

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637 *Code and Data Availability.* NLDAS-2 forcing is available from  
638 <https://ldas.gsfc.nasa.gov/nldas/v2/forcing>. SOIL and TOPO related datasets are downloaded  
639 from <https://svn-ccsm-inputdata.cgd.ucar.edu/trunk/inputdata/lnclm2/rawdata/>. LULC related  
640 datasets are from Ke et al. (2012); ERA5-Land reanalysis is available from:  
641 [https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land-monthly-](https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land-monthly-means?tab=overview)  
642 [means?tab=overview](https://cds.climate.copernicus.eu/cdsapp#!/dataset/reanalysis-era5-land-monthly-means?tab=overview). The ELM source code and surface data (e.g., SOIL, TOPO, LULC) used  
643 in this study are archived on Zenodo (<https://doi.org/10.5281/zenodo.6484857>).

644

645 *Author contributions.* LCL designed and conducted the experiments, analyzed model outputs, and  
646 drafted the manuscript. GB designed the study, interpreted the results, and improved the  
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649

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659

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661 **Reference**

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