1	Impacts of microtopographic snow-redistribution and lateral subsurface processes
2	on hydrologic and thermal states in an Arctic polygonal ground ecosystem : A case
3	study using ELM-3D v1.0
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5	Gautam Bisht <sup>1</sup> , William J. Riley <sup>1</sup> , Haruko M. Wainwright <sup>1</sup> , Baptiste Dafflon <sup>1</sup> , Yuan
6	Fengming <sup>2</sup> , and Vladimir E. Romanovsky <sup>3</sup>
7	
8	<sup>1</sup> Climate & Ecosystem Sciences Division, Lawrence Berkeley National Laboratory,1
9	Cyclotron Road, Berkeley, California 94720, USA
10	
11	<sup>2</sup> Environmental Sciences Division, Oak Ridge National Laboratory, Oak Ridge, TN, 37831-
12	6301 , USA
13	
14	<sup>3</sup> Geophysical Institute, University of Alaska Fairbanks, Fairbanks, AK 99775, USA
15	
16	Correspondence to: Gautam Bisht (gbisht@lbl.gov)
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18	Abstract
19	Microtopographic features, such as polygonal ground, are characteristic sources of
20	landscape heterogeneity in the Alaskan Arctic coastal plain. Here, we analyze the effects of
21	snow redistribution (SR) and lateral subsurface processes on hydrologic and thermal states
22	at a polygonal tundra site near Barrow, Alaska. We extended the land model integrated in
23	the E3SM to redistribute incoming snow by accounting for microtopography and
24	incorporated subsurface lateral transport of water and energy (ELM-3D v1.0). Multiple 10-
25	years long simulations were performed for a transect across polygonal tundra landscape at
26	the Barrow Environmental Observatory in Alaska to isolate the impact of SR and
27	subsurface process representation. When SR was included, model predictions better
28	agreed (higher R <sup>2</sup> , lower bias and RMSE) with observed differences in snow depth between
29	polygonal rims and centers. The model was also able to accurately reproduce observed soil
30	temperature vertical profiles in the polygon rims and centers (overall bias, RMSE, and $R^2$ of
31	0.59°C, 1.82°C, and 0.99, respectively). The spatial heterogeneity of snow depth during the

32 winter due to SR generated surface soil temperature heterogeneity that propagated in 33 depth and time and led to  $\sim 10$  cm shallower and  $\sim 5$  cm deeper maximum annual thaw 34 depths under the polygon rims and centers, respectively. Additionally, SR led to spatial 35 heterogeneity in surface energy fluxes and soil moisture during the summer. Excluding 36 lateral subsurface hydrologic and thermal processes led to small effects on mean states but 37 an overestimation of spatial variability in soil moisture and soil temperature as subsurface 38 liquid pressure and thermal gradients were artificially prevented from spatially dissipating 39 over time. The effect of lateral subsurface processes on maximum thaw depths was modest, 40 with mean absolute differences of  $\sim$ 3 cm. Our integration of three-dimensional subsurface 41 hydrologic and thermal subsurface dynamics in the E3SM land model will facilitate a wide 42 range of analyses heretofore impossible in an ESM context.

## 43 **1 Introduction**

44 The northern circumpolar permafrost region, which contains  $\sim 1700$  Pg of organic 45 carbon down to 3 m (Tarnocai et al., 2009), is predicted to experience disproportionately 46 larger future warming compared to the tropics and temperate latitudes (Holland and Bitz, 47 2003). Recent warming in the Arctic has led to changes in lake area (Smith et al., 2005), 48 snow cover duration and extent (Callaghan et al., 2011a), vegetation cover (Sturm et al., 49 2005), growing season length (Smith et al., 2004), thaw depth (Schuur et al., 2008), 50 permafrost stability (Jorgenson et al., 2006), and land-atmosphere feedbacks (Euskirchen 51 et al., 2009). Future predictions of Arctic warming include northward expansion of shrub 52 cover in tundra (Sturm et al., 2001; Tape et al., 2006), decreases in snow cover duration 53 (Callaghan et al., 2011a), and emissions of CO<sub>2</sub> and CH<sub>4</sub> from decomposition of 54 belowground soil organic matter (Koven et al., 2011; Schaefer et al., 2011; Schuur and 55 Abbott, 2011; Xu et al., 2016).

Several recent modeling studies have predicted a positive global carbon-climate
feedback at the global scale (Cox et al., 2000; Dufresne et al., 2002; Friedlingstein et al.,
2001; Fung et al., 2005; Govindasamy et al., 2011; Jiang et al., 2011; Jones et al., 2003;
Koven et al., 2015; Matthews et al., 2007a; Matthews et al., 2005; Sitch et al., 2008;
Thompson et al., 2004; Zeng et al., 2004), although the strength of this predicted feedback

at the year 2100 was shown to have a large variability across models (Friedlingstein et al.,
2006). In contrast to the ocean carbon cycle, the terrestrial carbon cycle is expected to be a
more dominant factor in the global carbon-climate feedback over the next century
(Matthews et al., 2007b; Randerson et al., 2015).

65 Snow, which covers the Arctic ecosystem for 8-10 months each year (Callaghan et 66 al., 2011b), is a critical factor influencing hydrologic and ecologic interactions (Jones, 67 1999). Snowpack modifies surface energy balances (via high reflectivity), soil thermal 68 regimes (due to low thermal conductivity), and hydrologic cycles (because of melt water). 69 Several studies have shown that warm soil temperatures under snowpack support the 70 emission of greenhouse gases from belowground respiration (Grogan and Chapin Iii, 1999; 71 Sullivan, 2010) and nitrogen mineralization (Borner et al., 2008; Schimel et al., 2004) 72 during winter. Additionally, decreases in snow cover duration have been shown to increase 73 net ecosystem CO<sub>2</sub> uptake (Galen and Stanton, 1995; Groendahl et al., 2007). Recent snow 74 manipulation experiments in the Arctic have provided evidence of the importance of snow 75 in the expected responses of Arctic ecosystems under future climate change (Morgner et al., 76 2010; Nobrega and Grogan, 2007; Rogers et al., 2011; Schimel et al., 2004; Wahren et al., 77 2005; Welker et al., 2000).

78 Apart from the spatial extent and duration of snowpack, the spatial heterogeneity of 79 snow depth is an important factor in various terrestrial processes (Clark et al., 2011; 80 Lundquist and Dettinger, 2005). As synthesized by López-Moreno et al. (2014), the 81 following processes are responsible for snow depth heterogeneity at three distinct spatial 82 scales: microtopography at 1-10 m (Lopez-Moreno et al., 2011); wind induced lateral 83 transport processes at 100-1000 m (Liston et al., 2007); and precipitation variability at 84 catchment scales of 10 – 1000 km (Sexstone and Fassnacht, 2014). The spatial distribution 85 of snow not only affects the quantity of snowmelt discharge (Hartman et al., 1999; Luce et 86 al., 1998), but also the water chemistry (Rohrbough et al., 2003; Wadham et al., 2006; 87 Williams et al., 2001). Lawrence and Swenson (2011) demonstrated the importance of 88 snow depth heterogeneity in predicting responses of the Arctic ecosystem to future climate 89 change by performing idealized numerical simulations of shrub expansion across the pan-90 Arctic region using the Community Land Model (CLM4). Their results showed that an 91 increase in active layer thickness (ALT), which is the maximum annual thaw depth, under

92 shrubs was negated when spatial heterogeneity in snow cover due to wind driven snow
93 redistribution was accounted for, resulting in an unchanged grid cell mean active layer
94 thickness.

95 Large portions of the Arctic are characterized by polygonal ground features, which 96 are formed in permafrost soil when frozen ground cracks due to thermal contraction 97 during winter and ice wedges form within the upper several meters (Hinkel et al., 2005). 98 Polygons can be classified as 'low-centered' or 'high-centered' based on the relationship 99 between their central and mean elevations. Polygonal ground features are dynamic 100 components of the Arctic landscape in which the upper part of ice-wedge thaw under low-101 centered polygon troughs leads to subsidence, eventually (~o(centuries)) converting the 102 low-centered polygon into a high-centered polygon (Seppala et al., 1991). Microtopography 103 of polygonal ground influences soil hydrologic and thermal conditions (Engstrom et al., 104 2005). In addition to controlling  $CO_2$  and  $CH_4$  emissions, soil moisture affects (1) 105 partitioning of incoming radiation into latent, sensible, and ground heat fluxes (Hinzman 106 and Kane, 1992; McFadden et al., 1998); (2) photosynthesis rates (McGuire et al., 2000; 107 Oberbauer et al., 1991; Oechel et al., 1993; Zona et al., 2011); and (3) vegetation

108 distributions (Wiggins, 1951).

109 Our goals in this study include (1) analyzing the effects of spatially heterogeneous 110 snow in polygonal ground on soil temperature and moisture and surface processes (e.g., 111 surface energy budgets); (2) analyzing how model predictions are affected by inclusion of 112 lateral subsurface hydrologic and thermal processes: and (3) developing and testing a 113 three-dimensional version of the E3SM Land Model (ELM; (Tang and Riley, 2016; Zhu and 114 Riley, 2015)), called ELM-3D v1.0 (hereafter ELM-3D). We then applied ELM-3D to a 115 transect across a polygonal tundra landscape at the Barrow Environmental Observatory in 116 Alaska. After defining our study site, the model improvements, model tests against 117 observations, and analyses, we apply the model to examine the effects of snow 118 redistribution and lateral subsurface processes on snow micro-topographical 119 heterogeneity, soil temperature, and the surface energy budget.

#### 120 2 Methodology

#### 121 **2.1 Study Area**

Our analysis focuses on sites located near Barrow, Alaska (71.3<sup>o</sup> N, 156.5<sup>o</sup> W) from 122 123 the long term Department of Energy (DOE) Next-Generation Ecosystem Experiment (NGEE-Arctic) project. The four primary NGEE-Arctic study sites (A, B, C, D) are located within the 124 125 Barrow Environmental Observatory (BEO), which is situated on the Alaskan Coastal Plain. 126 The annual mean air temperature for our study sites is approximately -13°C (Walker et al., 127 2005) and mean annual precipitation is 106 mm with the majority of precipitation 128 occurring during the summer season (Wu et al., 2013). The study site is underlain with 129 continuous permafrost (Brown et al., 1980) and the annual maximum thaw depth (active layer depth) ranges between 30-90 cm (Hinkel et al., 2003). Although the overall 130 131 topographic relief for the BEO is low, the four NGEE study sites have distinct 132 microtopographic features: low-centered (A), high-centered (B), and transitional polygons 133 (C, D). Contrasting polygon types are indicative of different stages of permafrost 134 degradation and were the primary motivation behind the choice of study sites for the 135 NGEE-Arctic project. LIDAR Digital Elevation Model (DEM) data were available at 0.25 m 136 resolution for the region encompassing all four NGEE sites. In this work, we perform 137 simulations along a two-dimensional transect in low-centered polygon Site-A as shown by 138 the dotted line in Figure 1.

#### 139 2.2 ELMv0 Description

The original version of ELM is equivalent to CLM4.5 (Ghimire et al., 2016; Koven et al., 2013; Oleson, 2013a), and represents vertical energy and water dynamics, including phase change. We developed ELM-3D by expanding on that model to explicitly represent soil lateral energy and hydrological exchanges and fine-resolution snow redistribution. We run ELM-3D here with prescribed plant phenology (called Satellite Phenology (SP) mode), since our focus is on thermal dynamics of the system, rather than C cycle dynamics.

#### 146 **2.3 Representing Two- and Three-Dimensional Physics**

- 147 **2.3.1** Subsurface hydrology
- 148 The flow of water in the unsaturated zone is given by the  $\theta$ -based Richards 149 equations as

$$\frac{\partial \theta}{\partial t} = -\nabla \cdot \vec{q} - Q \tag{1}$$

- 150 where  $\theta$  [m<sup>3</sup>m<sup>-3</sup>] is the volumetric soil water content, *t* [s] is time,  $\vec{q}$  [ms<sup>-1</sup>] is Darcy flux, and
- 151 Q [m<sup>-3</sup> of water m<sup>-3</sup> of soil s<sup>-1</sup>] is volumetric sink of water. Darcy flux is given by

$$\vec{q} = -k\nabla(\psi + z) \tag{2}$$

152 where *k* [ms<sup>-1</sup>] is the hydraulic conductivity,  $\psi$  [m] is the soil matric potential, and z [m] is

153 height above a reference datum. The hydraulic conductivity and soil matric potential are

154 non-linear functions of volumetric soil moisture. ELMv0 uses the modified form of Richards

equation of Zeng and Decker (2009) that computes Darcy flux as

$$\vec{q} = -k\nabla(\psi + z - C) \tag{3}$$

where C is a constant hydraulic potential above the water table,  $z_{\nabla}$ , given as

$$C = \psi_E + z = \psi_{sat} \left[ \frac{\theta_E(z)}{\theta_{sat}} \right]^{-B} + z = \psi_{sat} + z_{\nabla}$$
(4)

157 where  $\psi_E$  [m] is the equilibrium soil matric potential,  $\psi_{sat}$  [m] is the saturated soil matric 158 potential,  $\theta_E$  [m<sup>3</sup> m<sup>-3</sup>] is volumetric soil water content at equilibrium soil matric potential, 159  $\theta_{sat}$  [m<sup>3</sup> m<sup>-3</sup>] is volumetric soil water content at saturation,  $z_{\nabla}$  [m] is height of water table 160 above the reference datum, and *B* [-] is a fitting parameter for soil-water characteristic 161 curves. Substituting equations (3) and (4) into equation (1) yields the equation for the 162 vertical transport of water in ELMv0:

$$\frac{\partial \theta}{\partial t} = \frac{\partial}{\partial z} \left[ k \left( \frac{\partial (\psi - \psi_E)}{\partial z} \right) \right] - Q \tag{5}$$

- A finite volume spatial discretization and implicit temporal discretization with Taylor
   series expansion leads to a tri-diagonal system of equations. We extended this 1-D Richards
   equation to a 3-D representation integrated in ELM-3D, which is presented next.
- 166 We use a cell-centered finite volume discretization to decompose the spatial domain 167 into *N* non-overlapping control volumes,  $\Omega_n$ , such that  $\Omega = \bigcup_{n=1}^N \Omega_n$  and  $\Gamma_n$  represents the

boundary of the *n*-th control volume. Applying a finite volume integral to equation (1) andthe divergence theorem yields

$$\frac{\partial}{\partial t} \int_{\Omega_n} \theta dV = -\int_{\Gamma_n} \left( \vec{q} \cdot d\vec{A} \right) - \int_{\Omega_n} Q dV$$
(6)

170 The spatially discretized equation for the *n*-th grid cell that has  $V_n$  volume and n' neighbors 171 is given by

$$\frac{d\theta_n}{dt}V_n = -\sum_{n'} (\vec{q}_{nn'} \cdot \vec{A}_{nn'}) - QV_n \tag{7}$$

172 For the sake of simplicity in presenting the discretized equation, we assume the 3-D grid is

173 a Cartesian grid with each grid cell having a thickness of  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$  in the x, y, and z

- 174 directions, respectively. Using an implicit time integral, the 3-D discretized equation at time
- 175 t + 1 for a (i, j, k) control volume is given as

$$\left(\frac{\Delta\theta_{i,j,k}^{t+1}}{\Delta t}\right) V_{i,j,k} = \left(q_{x}_{i-1/2,j,k}^{t+1} - q_{x}_{i+1/2,j,k}^{t+1}\right) \Delta y \Delta z + \left(q_{y}_{i,j-1/2,k}^{t+1} - q_{y}_{i,j+1/2,k}^{t+1}\right) \Delta x \Delta z + \left(q_{z}_{i,j,k-1/2}^{t+1} - q_{z}_{i,j,k+1/2}^{t+1}\right) \Delta x \Delta y - Q V_{i,j,k}$$
(8)

176 where  $q_x$ ,  $q_y$  and  $q_z$  are Darcy flux in the x, y, and z directions, respectively and  $\Delta \theta_{i,j,k}^{t+1}$  is the 177 change in volumetric soil liquid water in time  $\Delta t$ . Using the same approach as Oleson 178 (2013b), the Darcy flux in all three directions is linearized about  $\theta$  using Taylor series 179 expansion. The linearized Darcy flux in the x direction at the (i - 1/2, j, k) interface is a 180 function of  $\theta_{i-1,j,k}$  and  $\theta_{i,j,k}$ :

$$q_{x_{i-1/2,j,k}}^{t+1} = q_{x_{i-1/2,j,k}}^{t} + \frac{\partial q_{x_{i-1/2,j,k}}^{t}}{\partial \theta_{i-1,j,k}} \Delta \theta_{i-1,j,k}^{t+1} + \frac{\partial q_{x_{i-1/2,j,k}}^{t}}{\partial \theta_{i,j,k}} \Delta \theta_{i+1,j,k}^{t+1}$$
(9)

The linearized Darcy fluxes in the *y* and *z* directions are computed similarly. Substituting
equation (9) in equation (8) results in a banded matrix of the form

$$\alpha \Delta \theta_{i-1,j,k}^{t+1} + \beta \Delta \theta_{i,j-1,k}^{t+1} + \gamma \Delta \theta_{i,j,k-1}^{t+1} + \eta \Delta \theta_{i+1,j,k}^{t+1} + \mu \Delta \theta_{i,j+1,k}^{t+1} + \phi \Delta \theta_{i,j,k+1}^{t+1}$$

$$+ \zeta \Delta \theta_{i,j,k}^{t+1} = \varphi$$

$$(10)$$

183 where  $\alpha$ ,  $\beta$ , and  $\gamma$  are subdiagonal entries;  $\eta$ ,  $\mu$ , and  $\phi$  are superdiagonal entries;  $\zeta$  is

184 diagonal entry of the banded matrix is given by

$$\alpha = \frac{\partial q_{x_{i-1/2,j,k}}}{\partial \theta_{i-1,j,k}} \Delta y \Delta z \tag{11}$$

$$\beta = \frac{\partial q_{y_{i,j-1/2,k}}}{\partial \theta_{i,j-1,k}} \Delta x \Delta z \tag{12}$$

$$\gamma = \frac{\partial q_{z_{i,j,k-1/2}}^{t}}{\partial \theta_{i,j,k-1}} \Delta x \Delta y \tag{13}$$

$$\eta = \frac{\partial q_{x_{i+1/2,j,k}}}{\partial \theta_{i+1,j,k}} \Delta y \Delta z \tag{14}$$

$$\mu = \frac{\partial q_{y_{i,j+1/2,k}}}{\partial \theta_{i,j+1,k}} \Delta x \Delta z \tag{15}$$

$$\phi = \frac{\partial q_{z_{i,j,k+1/2}}}{\partial \theta_{i,j,k+1}} \Delta x \Delta y \tag{16}$$

$$\zeta = \left(\frac{\partial q_{x_{i-1/2,j,k}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{x_{i+1/2,j,k}}}{\partial \theta_{i,j,k}}\right) \Delta y \Delta z + \left(\frac{\partial q_{y_{i,j-1/2,k}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{y_{i,j+1/2,k}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta z + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta y - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} + \left(\frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta y - \frac{\partial q_{z_{i,j,k}}}}{\partial x \Delta z} + \left(\frac{\partial q_{z_{i,j,k-1/2}}}}{\partial \theta_{i,j,k}} - \frac{\partial q_{z_{i,j,k-1/2}}}}{\partial \theta_{i,j,k}}\right) \Delta x \Delta y - \frac{\partial q_{z_{i,j,k-1/2}}}}{\partial x \Delta y} + \frac{\partial q_{z_{i,j,k}}}{\partial x \Delta y} + \frac{\partial q_{z_{i,j,k}}}}{\partial x \Delta y} + \frac{\partial q_{z_{i,j,k}}}{\partial x \Delta y} + \frac{\partial q_{z_{i,j,k}}}}{\partial x \Delta y} + \frac{\partial q_{z_{i,j,k}}}{\partial x \Delta y} + \frac{\partial q_{z_{i,j,k}}}}{\partial x \Delta y} + \frac{\partial q_{z_{i,j,k}}}{\partial x \Delta y} + \frac{\partial q_{z_$$

186 The column vector  $\varphi$  is given by

$$\varphi = -\left(q_{x_{i-\frac{1}{2},j,k}}^{t} - q_{x_{i+\frac{1}{2},j,k}}^{t}\right) \Delta y \Delta z - \left(q_{y_{i,j-\frac{1}{2},k}}^{t} - q_{y_{i,j+\frac{1}{2},k}}^{t}\right) \Delta x \Delta z$$

$$-\left(q_{z_{i,j,k-\frac{1}{2}}}^{t} - q_{z_{i,j,k+\frac{1}{2}}}^{t}\right) \Delta x \Delta y + Q_{i,j,k}^{t+1} \Delta x \Delta x \Delta z$$
(18)

187

The coefficients of equation (10) described in equation (11)-(18) are for an internal grid cell with six neighbors. The coefficients for the top and bottom grid cells are modified for infiltration and interaction with the unconfined aquifer in the same manner as Oleson (2013b). Similarly, the coefficients for the grid cells on the lateral boundary are modified for a no-flux boundary condition. See Oleson (2013b) for details about the computation of hydraulic properties and derivative of Darcy flux with respect to soil liquid water content.

#### 194 **2.3.2** Subsurface thermal

195 ELMv0 solves a tightly coupled system of equations for soil, snow, and standing
196 water temperature (Oleson, 2013a). The model solves the transient conservation of energy:

$$c\frac{\partial T}{\partial t} = -\nabla \cdot \mathbf{F} \tag{19}$$

where *c* is the volumetric heat capacity [J m<sup>-3</sup> K<sup>-1</sup>], F is the heat flux [W m<sup>-2</sup>], and t is time
[s]. The heat conduction flux is given by

$$F = -\lambda \nabla T \tag{20}$$

- 199 where  $\lambda$  is thermal conductivity [W m<sup>-1</sup> K<sup>-1</sup>] and T is temperature [K]. Applying a finite
- 200 volume integral to equation (20) and divergence theorem yields

$$c\frac{\partial}{\partial t}\int_{\Omega_n} T = -\int_{\Gamma_n} \vec{F} \cdot d\vec{A}$$
(21)

The spatially discretized equation for a *n*-th grid cell that has  $V_n$  volume and n' neighbors is given by

$$c_n \frac{dT_n}{dt} V_n = -\sum_{n'} \left( \vec{F}_{nn'} \cdot \vec{A}_{nn'} \right)$$
(22)

Similar to the approach taken in Section 2.3.1, ELM-3D assumes a 3-D Cartesian grid with

204 each grid cell having a thickness of  $\Delta x$ ,  $\Delta y$ , and  $\Delta z$  in the *x*, *y*, and *z* directions, respectively.

205 Temporal integration of equation (22) is carried out using the Crank-Nicholson method

that uses a linear combination of fluxes evaluated at time t and t + 1:

$$c_{n_{i,j,k}} \frac{\left(T_{i,j,k}^{t+1} - T_{i,j,k}^{t}\right)}{\Delta t} \Delta x \Delta y \Delta z$$

$$= \omega \left\{ \left(F_{x_{i-\frac{1}{2},j,k}}^{t} - F_{x_{i+\frac{1}{2},j,k}}^{t}\right) \Delta y \Delta z + \left(F_{y_{i,j-\frac{1}{2},k}}^{t} - F_{y_{i,j+\frac{1}{2},k}}^{t}\right) \Delta x \Delta z$$

$$+ \left(F_{z_{i,j,k-\frac{1}{2}}}^{t} - F_{z_{i,j,k+\frac{1}{2}}}^{t}\right) \Delta x \Delta y \right\}$$

$$+ (1 - \omega) \left\{ \left(F_{x_{i-\frac{1}{2},j,k}}^{t+1} - F_{x_{i+\frac{1}{2},j,k}}^{t+1}\right) \Delta y \Delta z$$

$$+ \left(F_{y_{i,j-\frac{1}{2},k}}^{t+1} - F_{y_{i,j+\frac{1}{2},k}}^{t+1}\right) \Delta x \Delta z$$

$$+ \left(F_{z_{i,j,k-\frac{1}{2}}}^{t+1} - F_{z_{i,j,k+\frac{1}{2}}}^{t+1} + 1\right) \Delta x \Delta y \right\}$$
(23)

- 207 where  $\omega$  is the weight in the Crank-Nicholson method and set to 0.5 in this study.
- 208 Substituting a discretized form of heat flux using equation (20) in equation (23), results in
- a banded matrix of the form

$$\alpha T_{i-1,j,k}^{t+1} + \beta T_{i,j-1,k}^{t+1} + \gamma T_{i,j,k-1}^{t+1} + \eta T_{i+1,j,k}^{t+1} + \mu T_{i,j+1,k}^{t+1} + + \phi T_{i,j,k+1}^{t+1} + \zeta \Delta T_{i,j,k}^{t+1} = \varphi$$
(24)

- 210 where  $\alpha$ ,  $\beta$ , and  $\gamma$  are subdiagonal entries;  $\eta$ ,  $\mu$ , and  $\phi$  are superdiagonal entries;  $\zeta$  is
- 211 diagonal entry of the banded matrix is given by

$$\alpha = \left(\frac{-(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta x}\right) \left(\frac{\lambda_{i-1/2,j,k}}{x_{i,j,k} - x_{i-1,j,k}}\right)$$
(25)

$$\beta = \left(\frac{-(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta y}\right) \left(\frac{\lambda_{i,j-1/2,k}}{y_{i,j,k}-y_{i-1,j,k}}\right)$$
(26)

$$\gamma = \left(\frac{-(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta z}\right) \left(\frac{\lambda_{i,j,k-1/2}}{z_{i,j,k}-z_{i,j,k-1}}\right)$$
(27)

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$$\eta = \left(\frac{-(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta x}\right) \left(\frac{\lambda_{i+1/2,j,k}}{x_{i+1,j,k}-x_{i,j,k}}\right)$$
(28)

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$$\mu = \left(\frac{-(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta y}\right) \left(\frac{\lambda_{i-1/2,j,k}}{y_{i+1,j,k}-y_{i,j,k}}\right)$$
(29)

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$$\phi = \left(\frac{-(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta z}\right) \left(\frac{\lambda_{i-1/2,j,k}}{z_{i+1,j,k}-z_{i,j,k}}\right)$$
(30)

$$\zeta = 1 + \left(\frac{(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta x}\right) \left[\frac{\lambda_{i-1/2,j,k}}{x_{i,j,k} - x_{i-1,j,k}} + \frac{\lambda_{i+1/2,j,k}}{x_{i+1,j,k} - x_{i,j,k}}\right] + \left(\frac{(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta y}\right) \left[\frac{\lambda_{i,j-1/2,k}}{y_{i,j,k} - y_{i-1,j,k}} + \frac{\lambda_{i-1/2,j,k}}{y_{i+1,j,k} - y_{i,j,k}}\right] + \left(\frac{(1-\omega)\Delta t}{c_{n_{i,j,k}}\Delta z}\right) \left[\frac{\lambda_{i,j,k-1/2}}{z_{i,j,k} - z_{i,j,k-1}} + \frac{\lambda_{i-1/2,j,k}}{z_{i+1,j,k} - z_{i,j,k}}\right]$$
(31)

219 The column vector  $\varphi$  is given by

220

$$\varphi = T_{i,j,k}^{t} + \left(\frac{\omega\Delta t}{c_{n_{i,j,k}}\Delta x}\right) \left(F_{x_{i-1/2,j,k}}^{t} - F_{x_{i+1/2,j,k}}^{t}\right) \\ + \left(\frac{\omega\Delta t}{c_{n_{i,j,k}}\Delta y}\right) \left(F_{y_{i,j-1/2,k}}^{t} - F_{y_{i,j+1/2,k}}^{t}\right) \\ + \left(\frac{\omega\Delta t}{c_{n_{i,j,k}}\Delta z}\right) \left(F_{z_{i,j,k-1/2}}^{t} - F_{z_{i,j,k+1/2}}^{t}\right)$$
(32)

221

222 The coefficients of equation (24) described in equation (25)-(32) are for an internal grid 223 cell with six neighbors. The coefficients for the top grid cells are modified for presence of 224 snow and/or standing water. A no-flux boundary condition was applied on the bottom grid 225 cells, thus no geothermal flux was accounted for in this study. The coefficients for the grid 226 cells on the lateral boundary are modified for a no-flux boundary condition. ELM handles 227 ice-liquid phase transitions by first predicting temperatures at the end of a time step and 228 then updating temperatures after accounting for deficits or excesses of energy during 229 melting or freezing. See Oleson (2013b) for details about the computation of thermal 230 properties and phase transition.

231

#### 2.3.3 PETSc Numerical solution

232 ELMv0, which considers flow only in the vertical direction, solves a tridiagonal and 233 banded tridiagonal system of equations for water and energy transport, respectively. In 234 ELM-3D, accounting for lateral flow in the subsurface results in a sparse linear system, 235 equations (10) and (24), where the sparcity pattern of the linear system depends on grid

cell connectivity. In this work, we use the PETSc (Portable, Extensible Toolkit for Scientific
Computing) library (Balay et al., 2016) developed at the Argonne National Laboratory to
solve the sparse linear systems. PETSc provides object-oriented data structures and solvers
for scalable scientific computation on parallel supercomputers. Description about the
numerical tests that were conducted to ensure the lateral coupling of hydrologic and
thermal processes was correctly implemented is presented in supplementary material
(Figure S 1 and S 2)

## 243 2.4 Snow Model and Redistribution

244 The snow model in ELM-3D is the same as that in the default ELMv0 and CLM4.5 245 (Anderson, 1976; Dai and Zeng, 1997; Jordan, 1991), except for the inclusion of snow 246 redistribution (SR). The snow model allows for a dynamic snow depth and up to five snow 247 layers, and explicitly solves the vertically-resolved mass and energy budgets. Snow aging, 248 compaction, and phase change are all represented in the snow model formulation. 249 Additionally, the snow model accounts for the influence of aerosols (including black and 250 organic carbon and mineral dust) on snow radiative transfer (Oleson, 2013a). ELMv0 uses 251 the methodology of Swenson and Lawrence (2012) to compute fractional snow cover area, 252 which is appropriate for ESM-scale grid cells (~100 km x 100 km). Since the grid cell 253 resolution in this work is sub-meter, we modified the fractional cover to be either 1 (when 254 snow was present) or 0 (when snow was absent).

255 Two main drivers of SR include topography and surface wind (Warscher et al., 256 2013); previous SR models include mechanistically- (Bartelt and Lehning, 2002; Liston and 257 Elder, 2006) and empirically- (Frey and Holzmann, 2015; Helfricht et al., 2012) based 258 approaches. To mimic the effects of wind, we used a conceptual model to simulate SR over 259 the fine-resolution topography of our site by instantaneously re-distributing the incoming 260 snow flux such that lower elevation areas (polygon center) receive snow before higher 261 elevation areas (polygon rims). This relatively simple and parsimonious approach is 262 reasonable given the observed snow depth heterogeneity, as described below, and small 263 spatial extent of our domain.

#### 264 **2.5 System Characterization**

265 Hydrologic and thermal properties differ by depth and landscape type. We used the 266 horizontal distribution of organic matter (OM) content from Wainwright et al. (2015) to 267 infer soil hydrologic and thermal properties following the default representations in ELM. 268 Vegetation cover was classified as arctic shrubs in polygon centers and arctic grasses in 269 polygon rims. The default representation of the plant wilting factor assigns a value of zero for a given soil layer when its temperature falls below a threshold (T<sub>threshold</sub>) of -2 <sup>o</sup>C. This 270 271 default value leads to overly large predicted latent and sensible heat fluxes during winter, 272 compared to nearby eddy covariance measurements. We modified T<sub>threshold</sub> to be 0 <sup>o</sup>C in this 273 study, resulting in improved predicted wintertime latent heat fluxes compared to the 274 default version of the model (Figure S3). Although biases compared to the observations 275 remain, particularly for sensible heat fluxes in the spring, the improvement is substantial 276 and, given the observational uncertainties, we believe sufficient to justify our use of the 277 model for investigations of the role of snow heterogeneity in this polygonal tundra system.

### 278 **2.6 Simulation Setup, Climate Forcing, and Analyses**

279 Because of computational constraints, we investigated the role of snow 280 redistribution and physics representation using a two-dimensional transect through site A 281 (Figure 1). The transect was 104 m long and 45 m deep and was discretized horizontally 282 with a grid spacing of 0.25 m and an exponentially varying layer thickness in the vertical 283 with 30 soil layers. The transect does not align with the sensor locations because our 284 objective was not to validate the model for a few grid cells, but to focus on relative 285 differences between predictions for rims and centers of a polygon field. No flow conditions 286 for mass and energy were imposed on the east, west, and bottom boundaries of the domain. 287 Temporal discretization of 30 min was used in the simulations. All simulations were 288 performed in the "satellite phenology" (SP) mode, i.e., Leaf Area Index (LAI) was prescribed 289 from MODIS observations.

Simulations were run for 10 years using long-term climate data gathered at the
Barrow, Alaska Observatory site (https://www.esrl.noaa.gov/gmd/obop/brw/) managed
by the Global Monitoring Division of NOAA's Earth System Research Laboratory (Mefford et
al., 1996). The missing precipitation time series was gap-filled using daily precipitation at

the Barrow Regional Airport available from the Global Historical Climatology Network
(<u>http://www1.ncdc.noaa.gov/pub/data/ghcn/daily</u>). We tested the model by comparing
predictions to high-frequency observations of snow depth and vertically resolved soil
temperature for September 2012 – September 2013. Temperature observations were
taken at discrete locations in a polygon center and rim (Figure 1), and were combined to
analyze comparable landscape positions in the simulations (Figure 2).

300 After testing, the model was used to investigate the effects of snow redistribution 301 and 2D subsurface hydrologic and thermal physics by analyzing three scenarios: (1) no 302 snow redistribution and 1D physics; (2) snow redistribution and 1D physics; and (3) snow 303 redistribution and 2D physics. Between these scenarios, we compared vertically-resolved 304 soil temperature and liquid saturation, active layer depth, and mean and spatial variation of 305 latent and sensible heat fluxes across the 10 years of simulations. For each soil column, the 306 simulated soil temperature was interpolated vertically and the active layer depth was 307 estimated as the maximum depth that had above-freezing soil temperature.

## 308 3 Results and Discussion

#### 309 **3.1 Snow depth**

310 In the absence of SR, predicted snow depth exactly follows the topography. With SR, 311 a much smaller dependence of winter-average snow depth on topography is predicted 312 (Figure 2). Further, for the winter average, there are very small differences in snow depth 313 between simulations with SR and 1D or 2D subsurface physics representations. Compared 314 to observations, considering SR led to: (1) a factor of  $\sim 2$  improvement in snow depth bias 315 for the polygon center; (2) modest increase and decrease in average bias on the rims for 316 September through February and March through June, respectively; and (3) a dramatic 317 improvement in bias of the difference in snow depth between the polygon centers and rims 318 (Figure 3). There was no discernible difference in snow depth bias between the 1D and 2D 319 physics (Table 1), although the predicted subsurface temperature fields were different, as 320 shown below.

The temporal variation of the mean snow depth (**Figure 4**a) and its spatial standard deviation (**Figure 4**b) also differed based on whether SR was considered, but was not affected by considering 2D thermal or hydrologic physics. With SR, the snow depth
coefficient of variation (Figure 4c) was about 0.5 from December through the beginning of
the snowmelt period, indicating relatively large spatial heterogeneity. Simulated snow
depth for the three simulation scenarios are included in Supplementary Material (4)

#### **327 3.2 Soil Temperature and Active Layer Depth**

328 Broadly, ELM-3D accurately predicted the polygon center soil temperature at depth 329 intervals corresponding to the temperature probes (0-20 cm, 20-50 cm, 50-75 cm, and 75-330 100 cm; Figure 5a). Recall that the observed temperatures for the polygon center and rims 331 were taken at single points in site A (Figure 1) while the predicted temperatures were 332 calculated as averages across the transect for each of the two landscape position types. The 333 model was able to simulate early freeze up of the soil column under the rims as compared 334 to centers in November 2012 because of differences in accumulated snow pack. The 335 transition to thawed soil in the 0-20 cm depth interval in early June 2013 and the 336 subsequent temperature dynamics over the summer were very well captured by ELM-3D. 337 Minimum temperatures during the winter were also accurately predicted, although the 338 temperatures in the deepest layer (75-100 cm) were overestimated by  $\sim$ 3°C in March. For 339 figure clarity we did not indicate the standard deviation of the observations, but provide 340 that information in Supplemental Material (Figure S5-S8).

Similarly, the soil temperatures were accurately predicted in the polygon rims (Figure 5b). The largest discrepancies between measured and predicted soil temperatures were in the shallowest layer (0 - 25 cm), where the predictions were up to a few °C cooler than some of the observations between December 2012 and March 2013. In the polygon center, a thicker snow pack acts as a heat insulator and keeps soil temperature higher in winter as compared to the polygon rims.

Three recent studies have used other mechanistic models to simulate soil temperature fields at this site, and achieved comparably good comparisons with observations (Kumar et al. 2016 applied a 3D version of PFLOTRAN; Atchley et al. 2015 and Harp et al. 2016 applied a 1D version of ATS). However, those models used measured soil temperatures near the surface as the top boundary condition. In contrast, the top boundary condition in this work is the climate forcing (air temperature, wind, solar radiation,

humidity, precipitation), and the ground heat flux is prognosed based on ELM's vegetation
and surface energy dynamics. We note that no parameter calibration was done in this work
or that of Kumar et al. (2016), while the ATS parameterizations were calibrated to match
the soil temperature profile.

Snow redistribution impacts spatial variability of soil temperature throughout the soil column. Absence of SR results in no significant spatial variability of soil temperature (Figure 6a). Inclusion of SR on the surface modifies the amount of energy exchanged between the snow and the top soil layer, thereby creating spatial variability in the temperature of the top soil, which propagates down into the soil column (Figure 6b). With SR, energy dissipation in the lateral direction reduces the penetration depth of the soil temperature spatial variance (compare Figure 6c and Figure 6b).

364 With 1D physics, the average spatial and temporal difference of the active layer 365 depth (ALD) between simulations with and without SR was 1.7 cm (Figure 7a), and the 366 absolute difference was 6.5 cm. As described above, we diagnosed the ALD to be the 367 maximum soil depth during the summer at which vertically interpolated soil temperature 368 is 0 °C. On average, the rims had  $\sim$ 10 cm shallower ALD with (blue line) than without 369 (green line) SR, consistent with the loss of insulation from SR on the rims during the 370 winter. In the centers (e.g., at location 42 - 55 m), the thaw depth was deeper by  $\sim$ 5 cm 371 with SR because of the higher snow depth there from SR. The effect of SR on the ALD was 372 largest on the rims because, compared to centers, they (1) on average lost more snow with 373 SR and (2) are more thermally conductive. Since rims are therefore colder at the time of 374 snowmelt with SR, the ground heat flux during the subsequent summer was unable to thaw 375 the soil column as deeply as when SR is ignored. For comparison, Atchley et al. (2015) found in their sensitivity analysis using the 1D version of ATS that SR resulted in deeper 376 377 thaw depths in both polygon centers (by  $\sim$ 3 cm) and rims ( $\sim$ 0.3 cm). Thus, their results for 378 polygon centers are consistent in sign but lower in magnitude than ours, but opposite in 379 sign for the rims.

Across ten years of simulation, the inter-annual variability (IAV) in ALD varied substantially between the three scenarios (Figure 7b). As expected, for the 1D physics without SR scenario (green line), the IAV in ALD was determined by landscape position because of differences in soil and vegetation parameters. With SR and 1D physics, the

model shows largest differences over the rims, again highlighting the relatively larger
effects of SR on the rim soil temperatures.

The effect of 1D versus 2D physics on the ALD across the transect was modest (mean absolute difference ~3 cm). Generally, because 2D physics allows for lateral energy diffusion, the horizontal variation of ALD was slightly lower (i.e., the red line is smoother than the blue line; Figure 7a) than with 1D physics. This difference was also reflected in the thaw depth IAV across the transect, where 2D physics led to a smoother lateral profile of inter-annual variability than with 1D physics.

392 The impact of physics formulation (i.e., 1D or 2D) alone was investigated by 393 analyzing differences between soil temperature profiles over time for polygon rims and 394 centers in simulations with snow redistribution. Inclusion of 2D subsurface physics 395 resulted in soil temperatures with depth and time that were lower in the polygon rims 396 (Figure 8a) and higher in polygon centers (Figure 8b). Using the simulations from the 397 scenario with SR and 2D physics, we evaluated the extent to which soils under rims and 398 centers can be separately considered as relatively homogeneous single column systems by 399 evaluating the soil temperature standard deviation as a function of depth and time (Figure 400 9). During winter, both polygon rims and centers were predicted to have soil temperature spatial variability >1  $^{\circ}$ C up to a depth of ~2 m. The soil temperature spatial variability in 401 402 winter due to snow redistribution was dissipated over the summer. During the summer, 403 polygon centers were relatively more homogeneous vertically compared to polygon rims.

## 404 **3.3** Surface Energy Budget

405 Predicted monthly- and spatial-mean  $(\mu)$  surface latent heat fluxes across the 406 transect were very similar between the three scenarios (Figure 10a), with a growing 407 seasonal mean difference of < 1.0 W m<sup>-2</sup>. However, the spatial variability (SV =  $\sigma$ ; Figure 408 10b) and coefficient of variation (CV =  $\sigma/\mu$ ; Figure 10c) of latent heat fluxes were different 409 between the scenarios with SR (1D and 2D physics) and without SR. With SR, the latent 410 heat flux spatial standard deviation peaked after snowmelt and declined until the fall when 411 snow began, from about  $\sim 100\%$  to 10% of the mean. This relatively larger spatial variation 412 in latent heat flux occurred because of large spatial heterogeneity in near surface soil

413 moisture in the beginning of summer, indicating a residual effect of SR from the previous414 winter.

415 The predicted temporal monthly-mean and spatial-mean surface sensible heat 416 fluxes across the transect were also similar between the three scenarios (Figure 11a), with 417 a growing season mean absolute difference of < 3.5 W m<sup>-2</sup>. Also, the sensible heat flux 418 spatial variability differences occurred earlier than snowmelt, in contrast to the latent heat 419 flux. Both the standard deviation and CV of the sensible heat fluxes were larger than those 420 of the latent heat fluxes, with early season standard deviations of  $\sim 50$  W m<sup>-2</sup> (Figure 11b) 421 and CV's of  $\sim$ 1.5 (Figure 11c). As for the latent heat fluxes, the differences in standard 422 deviation and CV of sensible heat fluxes were small between the 1D and 2D scenarios with 423 SR, arguing that the subsurface lateral energy exchanges associated with the 2D physics did 424 not propagate to the mean surface heat fluxes. However, as for the latent heat flux, there 425 was a relatively large difference in spatial variation between the scenarios with and 426 without SR (e.g., of about 25 W  $m^{-2}$  in May; Figure 10b).

#### 427 **3.4 Soil Moisture**

428 Neither SR nor 2D lateral physics affected the spatial mean moisture across time 429 (not shown). However, spatial heterogeneity of predicted soil moisture content differed 430 substantially between scenarios during the snow free period (Figure 12). For the 1D 431 simulations, the effect of SR was to increase growing season soil moisture spatial 432 heterogeneity by factors of 5.2 and 1.6 for 0-10 cm and 10-65 cm depth intervals, 433 respectively (compare Figure 12a and Figure 12b). Compared to 1D physics, simulating 2D 434 thermal and hydrologic physics led to an overall reduction in soil moisture spatial 435 heterogeneity by factors of 0.8 and 0.7 for 0-10 cm and 10-65 cm depth intervals, 436 respectively (compare Figure 12b and Figure 12c). Thus, with respect to dynamic spatial 437 mean soil moisture, SR effects dominated those associated with lateral subsurface water 438 movement.

### 439 **3.5 Caveats and Future Work**

The good agreement between ELM-3D predictions and soil temperature
observations demonstrate the model's capabilities to represent this very spatially

heterogeneous and complex system. However, several caveats to our conclusions remain
due to uncertainties in model parameterizations, model structure, and climate forcing data.

444 ELMv0, a one-dimensional model, is embarrassing parallel with no cross processor 445 communication. The current implementation of the three-dimensional solver in ELM-3D 446 only supports serial computing. Support of parallel computing will be included in a future 447 version of the model. Because of computational constraints, we applied a 2D transect 448 domain to the site, instead of a full 3D domain. We are working to improve the 449 computational efficiency of the model, which will facilitate a thorough analysis of the 450 effects of 3D subsurface energy and water fluxes. A related issue is our simplified treatment 451 of surface water flows. A thorough analysis of the effects of surface water redistribution 452 would require integration of a 2D surface thermal flow model in a 3D domain, which is 453 another goal for our future work. However, we note that the good agreement using the 2D 454 model domain supports the idea that a two-dimensional simplification may be appropriate 455 for this system. The expected geomorphological changes in these systems over the coming 456 decades (e.g., Liljedahl et al. 2016), which will certainly affect soil temperature and 457 moisture, are not currently represented in ELM, although incorporation of these processes 458 is a long-term development goal.

459 The current representation of vegetation in ELM-3D for these polygonal tundra 460 systems is over-simplified. For example, non-vascular plants (mosses and lichens) are not 461 explicitly represented in the model, but can be responsible for a majority of evaporative 462 losses (Miller et al., 1976) and are strongly influenced by near surface hydrologic 463 conditions (Williams and Flanagan, 1996). Our use of the 'satellite phenology' mode, which 464 imposes transient LAI profiles for each plant functional type in the domain, ignores the 465 likely influence of nutrient constraints (Zhu et al., 2016) on photosynthesis and therefore 466 the surface energy budget. Other model simplifications, e.g., the simplified treatment of 467 radiation competition may also be important, especially as simulations are extended over 468 periods where vegetation change may occur (e.g., Grant 2016).

Development of sub grid parameterizations to parsimoniously capture fine scale
processes will be pursued in the future. For example, a two-tile approach to represent
hydrologic and thermal processes in coupled polygon rims and centers with snow
redistribution should be evaluated. Inclusion of lateral subsurface processes has a greater

473 impact on predicted subgrid variability than on spatially averaged states. Thus, one 474 possible extension of the current model would be to explicitly include an equation for the 475 temporal evolution of sub grid variability using the approach of Montaldo and Albertson 476 (2003). The use of reduced-order models (e.g., Pau et al. (2014); Liu et al. (2016)) is an 477 alternate approach to estimate fine scale hydrologic and thermal states from a coarse 478 resolution representation. Additionally, lateral subsurface processes can be included in the 479 land surface model via a range of numerical discretization approaches of varying 480 complexity, e.g., adding lateral water and energy fluxes as source/sink terms in the existing 481 1D model, implementing an operator split approach to solve vertical and lateral processes 482 in a non-iterative approach, or solving a fully coupled 3D model. Tradeoffs between 483 approaches that represent lateral processes and computational costs need to be carefully 484 studied before developing quasi or fully three-dimensional land surface models. While the 485 present study focused on application and validation of ELM-3D at fine-scale, future work 486 will focus on regional scale applications using comprehensive datasets and the Distributed 487 Model Intercomparison Project Phase 2 modeling protocol (Smith et al., 2012). Although 488 we found no significant effect of topography and SR on the 100 m  $\times$  100 m grid-averaged 489 exchanges with the atmosphere, future work needs to analyze intermediate scale (e.g., 100 490 m – 10 km) topographical variation and the potential effects on biogeochemical and plant 491 processes and surface exchanges.

## 492 **4 Summary and Conclusions**

In a polygonal tundra landscape, we analyzed effects of microtopographical surface heterogeneity and lateral subsurface transport on soil temperature, soil moisture, and surface energy exchanges. Starting from the climate-scale land model ELMv0, we incorporated in ELM-3D numerical representations of subsurface water and energy lateral transport that are solved using PETSc. A simple method for redistributing incoming snow along the microtopographic transect was also integrated in the model.

Over the observational record, ELM-3D with snow redistribution and lateral heat and hydrological fluxes accurately predicted snow depth and soil temperature vertical profiles in the polygon rims and centers (overall bias, RMSE, and R<sup>2</sup> of 0.59°C, 1.82°C and 502 0.99, respectively). In the rims, the transition to thawed soil in spring, summer 503 temperature dynamics, and minimum temperatures during the winter were all accurately 504 predicted. In the centers, a  $\sim 2^{\circ}$ C warm bias in April in the 75-100 cm soil layer was 505 predicted, although this bias disappeared during snowmelt.

506 The spatial heterogeneity of snow depth during the winter due to snow 507 redistribution generated surface soil temperature heterogeneity that propagated into the 508 soil over time. The temporal and spatial variation of snow depth was affected by snow 509 redistribution, but not by lateral thermal and hydrologic transport. Both snow 510 redistribution and lateral thermal fluxes affected spatial variability of soil temperatures. 511 Energy dissipation in the lateral direction reduced the depth to which soil temperature 512 variance penetrated. Snow redistribution led to  $\sim 10$  cm shallower active layer depths 513 under the polygon rims because of the residual effect of reduced insulation during the 514 winter. In contrast, snow redistribution led to  $\sim$ 5 cm deeper maximum thaw depth under 515 the polygon centers. The effect of lateral energy fluxes on active layer depths was  $\sim 3$  cm. 516 Compared to 1D physics, the 2D subsurface physics led to lower (higher) soil temperatures 517 with depth and time in the polygon rims (centers). The larger than 1 °C wintertime spatial 518 temperature variability down to  $\sim 2$  m depth in rims and centers indicates the uncertainty 519 associated with considering rims and centers as separate 1D columns. During the summer, 520 polygon center temperatures were relatively more vertically homogeneous than 521 temperatures in the rims.

522 The monthly- and spatial-mean predicted latent and sensible heat fluxes were 523 unaffected by snow redistribution and lateral heat and hydrological fluxes. However, snow 524 redistribution led to spatial heterogeneity in surface energy fluxes and soil moisture during 525 the summer. Excluding lateral subsurface hydrologic and thermal processes led to an over 526 prediction of spatial variability in soil moisture and soil temperature because subsurface 527 gradients were artificially prevented from laterally dissipating over time. Snow 528 redistribution effects on soil moisture heterogeneity were larger than those associated 529 with lateral thermal fluxes.

530 Overall, our analysis demonstrates the potential and value of explicitly representing 531 snow redistribution and lateral subsurface hydrologic and thermal dynamics in polygonal 532 ground systems and quantifies the effects of these processes on the resulting system states and surface energy exchanges with the atmosphere. The integration of a 3D subsurface
model in the E3SM Land Model also allows for a wide range of analyses heretofore
impossible in an Earth System Model context.

# 537 **5 Code availability**

- 538 The ELM-3D v1.0 code and data used in study are publicly available at
- 539 https://bitbucket.org/gbisht/lateral-subsurface-model and
- 540 https://bitbucket.org/gbisht/notes-for-gmd-2017-71.
- 541

## 542 **6 Tables**

- 543 Table 1. Bias, root mean square error (RMSE), and correlation (R<sup>2</sup>) between modeled and
- 544 observed snow depth at polygon center, rim and difference between center and rim for
- 545 2013 for three cases: Snow redistribution (SR) off and 1D physics, SR on and 1D physics,
- 546 and SR on and 2D physics.

	SR=Off, Physics=1D			SR=On, Physics=1D			SR=On, Physics=2D		
	Center Rim Center-		Center Rim Center-		Center Rim		Center-		
			Rim			Rim			Rim
Bias	-0.08	0.02	-0.10	-0.04	-0.03	-0.02	-0.04	-0.03	-0.02
RMSE	0.12	0.04	0.12	0.08	0.04	0.05	0.08	0.04	0.05
R <sup>2</sup>	0.86	0.92	0.03	0.78	0.85	0.73	0.79	0.85	0.73

547

- 549 Table 2 Bias, root mean square error (RMSE) and correlation (R<sup>2</sup>) between modeled and
- **observed soil temperature at polygon center and rim at multiple soil depth for 2013 for**
- 551 three cases: Snow redistribution (SR) off and 1D physics, SR on and 1D physics, and SR on
- 552 and 2D physics.

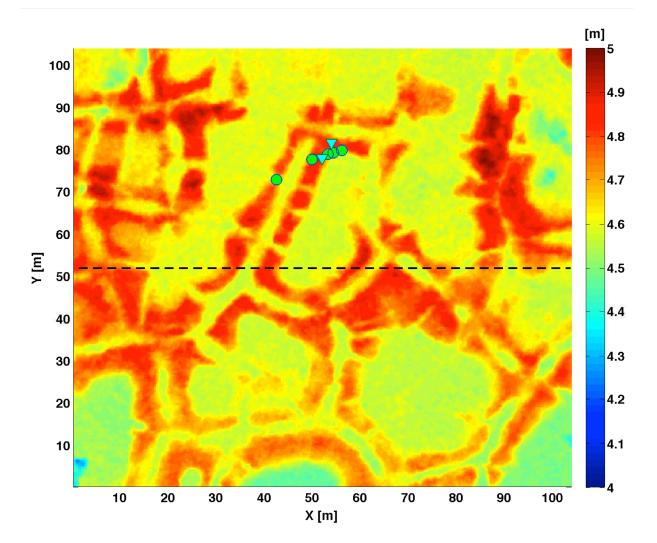
Bias								
	SR=Off, Physics=1D		SR=On, Ph	ysics=2D	SR=On, Physics=2D			
Depth [m]	Center	Rim	Center	Rim	Center	Rim		
0.00 - 0.20	0.86	-1.73	-0.19	1.00	0.52	0.71		
0.20 - 0.50	0.68	-1.52	-0.46	0.98	0.35	0.62		
0.50 - 0.75	0.53	-1.49	-0.64	0.94	0.21	0.53		
0.75 - 1.00	0.49	-1.44	-0.67	-0.97	0.22	0.49		
Average across four depths	0.64	-1.54	-0.49	0.97	0.33	0.59		

RMSE								
	SR=Off, P	hysics=1D	SR=On, Pł	nysics=2D	SR=On, Physics=2D			
Depth [m]	Center	Rim	Center	Rim	Center	Rim		
0.00 - 0.20	2.11	3.39	2.20	2.94	1.90	2.66		
0.20 - 0.50	1.49	2.73	1.39	1.86	1.12	1.57		
0.50 - 0.75	1.60	2.42	1.22	1.96	1.14	1.60		
0.75 - 1.00	1.50	2.15	1.12	1.87	1.09	1.44		
Average	1.67	2.67	1.44	2.16	1.31	1.82		
across four								
depths								

R <sup>2</sup>									
	SR=Off, Physics=1D SR=On, Physics=2D SR=On, Physics=2D								
Depth [m]	Center	Rim	Center	Rim	Center	Rim			
0.00 - 0.20	0.98	0.95	0.97	0.97	0.98	0.97			

0.20 - 0.50	0.99	0.96	0.98	0.99	0.99	0.99
0.50 - 0.75	0.99	0.97	0.99	0.99	1.00	0.99
0.75 - 1.00	0.99	0.97	0.99	0.99	1.00	0.99
Average	0.99	0.96	0.98	0.99	0.99	0.99
across four						
depths						

## 557 **7 Figures**



558

Figure 1 The NGEE-Arctic study area A, which characterized as a low-centered polygon field. Dotted line indicate the transect along which simulation in this paper are preformed to demonstrate the effects of snow redistribution on soil temperature. The locations where snow and temperature sensors are installed within the study site are denoted by triangle and circle, respectively.

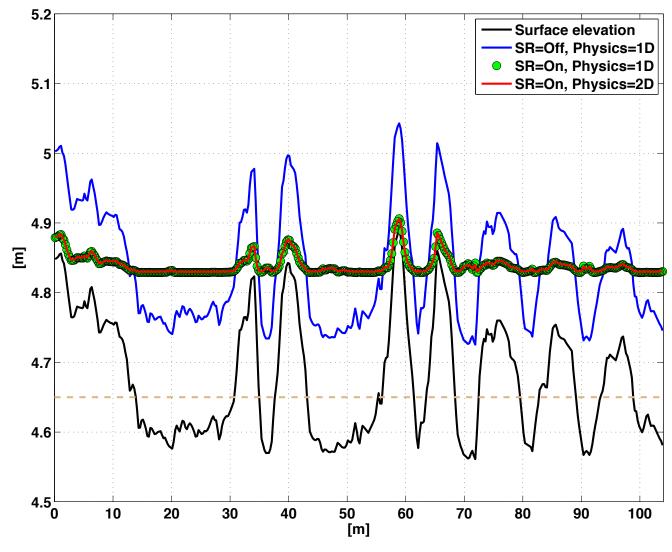


Figure 2. Simulated average winter snow surface elevation across the transect for three scenarios: (1) snow redistribution (SR) turned off and 1D subsurface physics, (2) snow redistribution turned on and 1D subsurface physics, and (3) snow redistribution turned on and 2D subsurface physics. Surface elevation of the transect is shown by solid black line. The dashed line indicates the boundary for comparison to observations in relatively lower (centers) and relatively higher (rims) topographical positions.

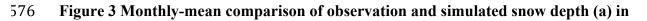
(a) Snow depth in polygon rim Obs. SR=Off, Physics=1D 0.4 SR=On, Physics=1D Ξ SR=On, Physics=2D 0.2 œ (b) Snow depth in polygon center 0.6 0.4 Ξ 0.2 0 (c) Difference in snow depth between polygon center and rim 0.4 <u></u> E 0.2

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577 polygon rim, (b) in polygon center; (c) difference between polygon center and rim for 2013.

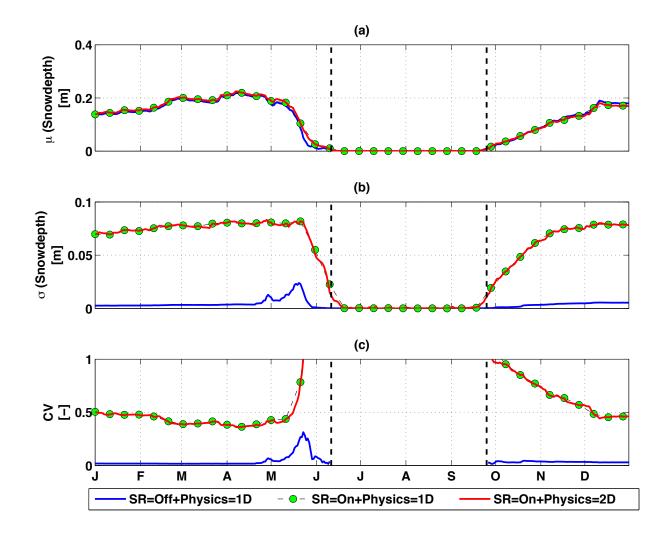
F

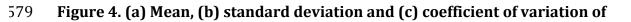
Μ

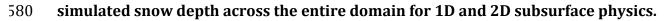
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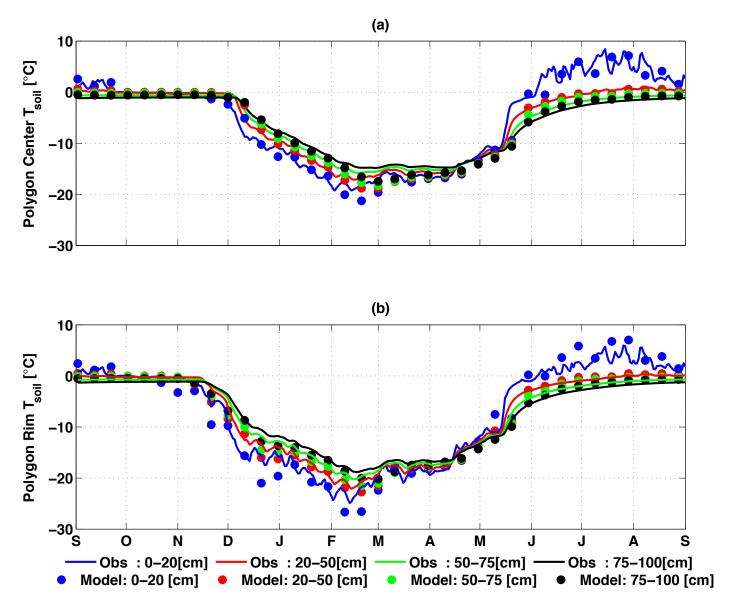


Figure 5 Comparison of soil temperature observations and predictions in polygon centers (a) and rims (b). Simulation was performed with snow redistribution on and 2D subsurface physics, between September 2012 and September 2013. Simulation results are shown at an interval of 10 days, while observations are shown at daily interval

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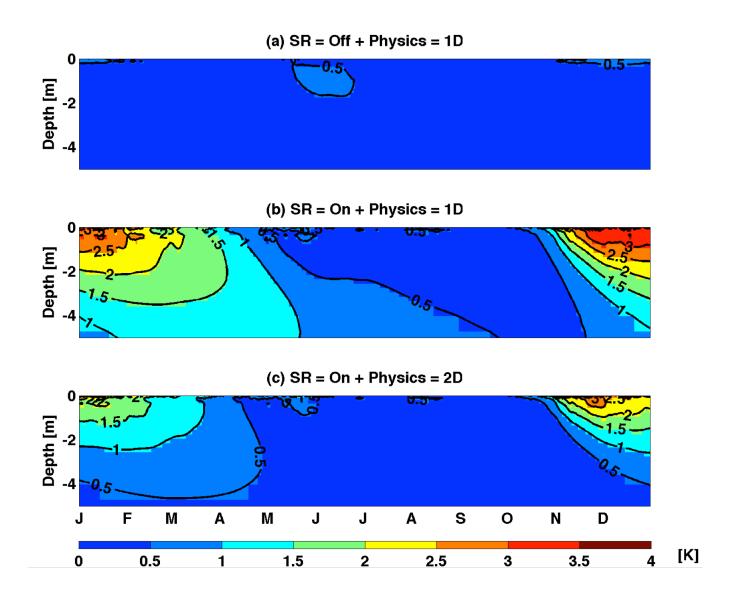


Figure 6 Simulated daily spatial standard deviation for each soil layer averaged across 10year of near surface soil temperature for simulation performed with snow redistribution turned off and 1D subsurface physics (top panel); snow redistribution turned on and 1D subsurface physics (middle panel); and snow redistribution turned on and 2D subsurface physics (bottom panel).

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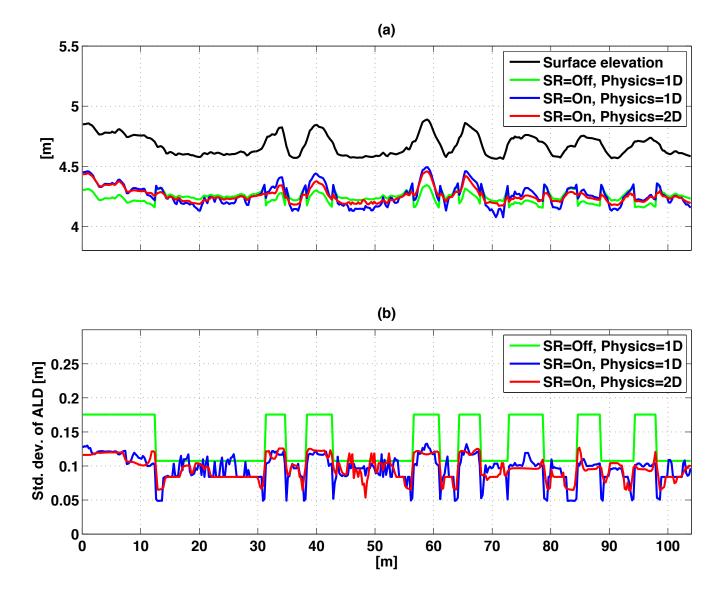
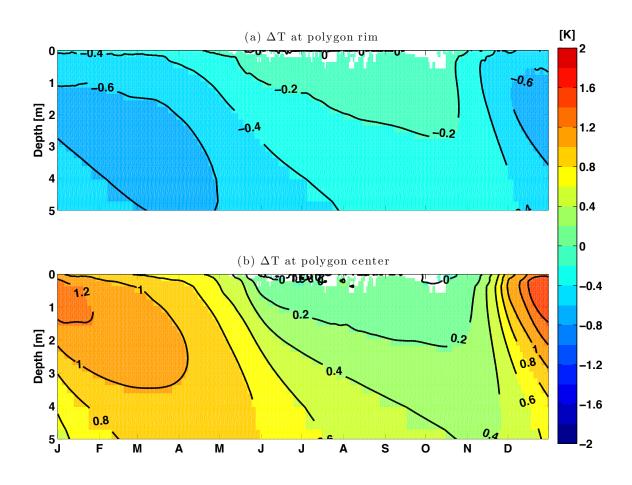
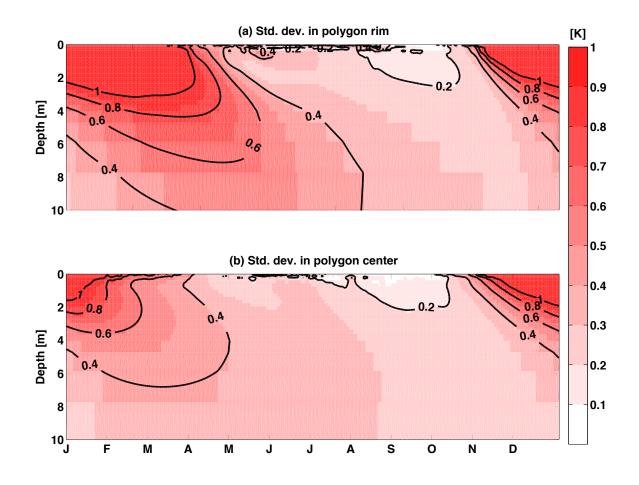


Figure 7 Temporal mean of the bottom of the active layer (top panel) and standard
deviation of the active layer depth (bottom panel) over the 10-year period across the
modeling domain.

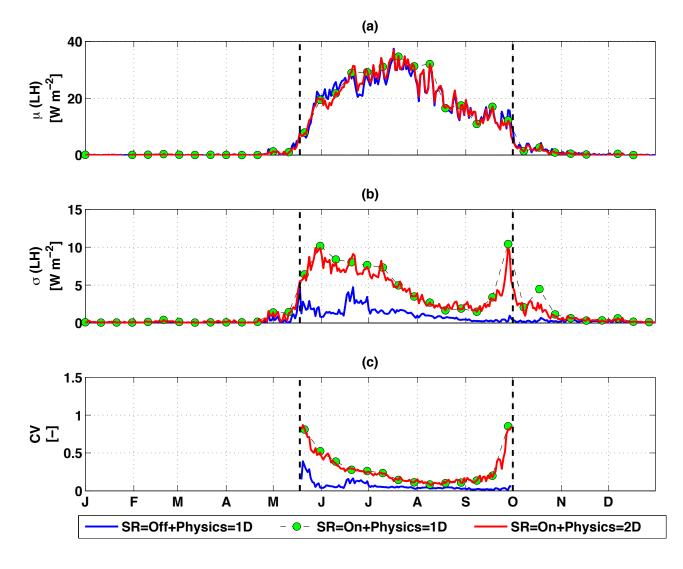




- 505 Figure 8 Time series of spatial mean soil temperature differences between "SR=On +
- **Physics=1D" and "SR=On + Physics=2D" at polygon rim (top panel) and polygon center**
- 507 (bottom panel).

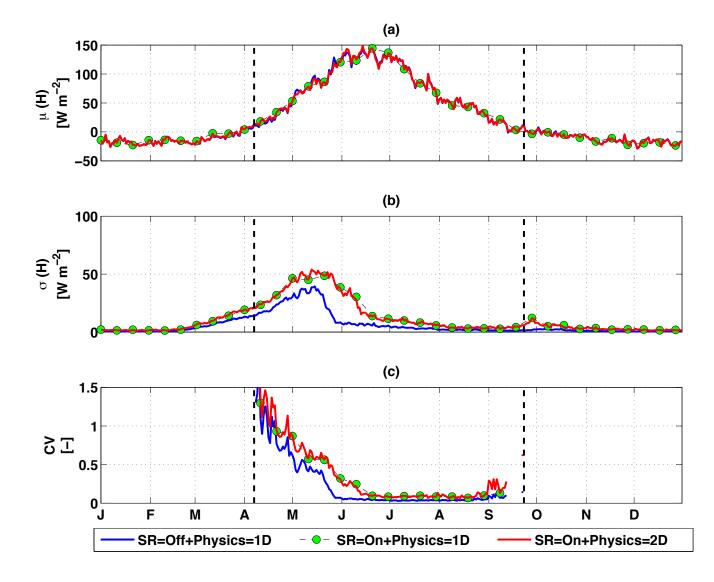


- 509 Figure 9 Time series of soil temperature spatial standard deviation for "SR=On +
- 510 Physics=2D" at polygon rim (top panel) and polygon center (bottom panel).

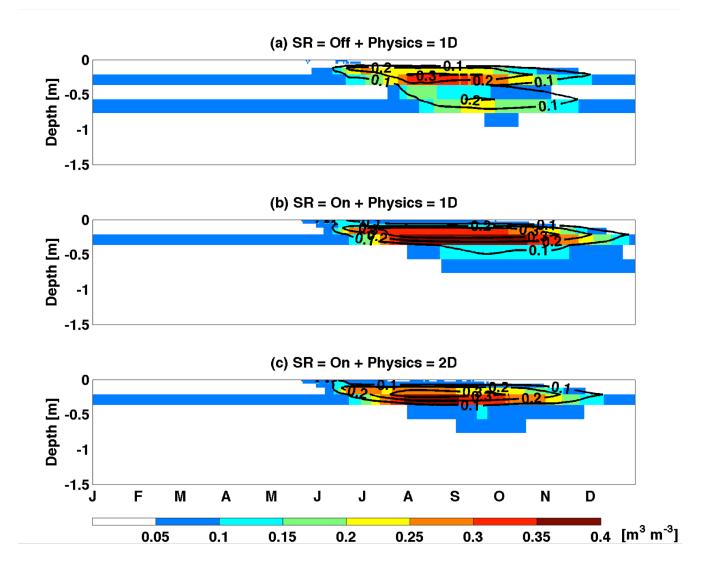




coefficient of variation across the site A transect.







521 Figure 12. Same as Figure 6 except for liquid saturation.

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