The New Prognostic Canopy Air Space Solution in the Community Land Model Version 4 (CLM4)

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Preface

The present document describes the update to an analytical method of solving for variables near the land-atmosphere interface that will appear in the Community Land Model version 4 (CLM4). This document is an addendum to the standard CLM technical description (Oleson *et al.* 2004). This work was supported in part by the … program through grant ….

Samuel Levis

Boulder, 7 March 2006

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1. Introduction

The Community Land Model (CLM) solves a set of simultaneous equations once per model time step *n*. The unknowns in this set of equations include near-surface prognostic temperature and humidity variables for time step $n + 1$.

The near-surface state responds to the conditions prescribed by an atmospheric data set when the CLM operates in offline mode or simulated by an atmospheric general circulation model (GCM) when the CLM operates in coupled mode. In the latter case, CLM's calculated sensible and latent heat fluxes are passed to the GCM to establish two-way land-atmosphere interactions.

CLM versions prior to version 4 employ an iterative scheme of solving for near-surface temperature and humidity (Oleson *et al.* 2004). Here we document the model update to an analytical method of solving for the same variables using a matrix solver. This update will appear in CLM version 4. The analytical solution of this matrix of equations will simplify large sections of the code and will allow for an easier implementation of water isotope tracers in CLM.

The CLM already solves a set of soil and snow temperature and moisture equations using a matrix solver. In CLM version 4 the soil and snow temperature equations will be solved as part of the new matrix, while the moisture equations will continue to be solved in a separate matrix.

2. The Equations and their Physical Basis

This section includes subsections numbered by matrix row, where each row corresponds to an equation. All rows together form the simultaneous set of equations solving for a number of unknowns equal to the number of equations. The complete matrix appears in section 3. Symbols for all variables are consistent with Oleson *et al.* (2004).

Each equation is presented in three forms: (a) the physical form, (b) a series of forms following algebraic transformations, and (c) the matrix coefficient form. The algebraic transformations assume an "explicit coefficient/implicit temperature" numerical scheme (Kalnay and Kanamitsu 1988). "Explicit coefficient" means that we use the resistance terms (r_{ah}, r_{aw}, r_b) calculated at time step n, while "implicit temperature" means that the variables on the right hand side (RHS) of the equations are from time step $n + 1$.

2.1 Solving for T_s

Eq. 1 solves for T_s (K), the canopy air space temperature. Eq. 1 states that the change in T_s per time increment Δt (s) between time steps n and $n + 1$ is directly proportional to the sum of sensible heat fluxes (W m^{-2}) from the ground, H_g, the vegetation, H_v, and the GCM's reference height ($z_{atm,h} \approx 30$ m above the ground), H, to the height of the canopy air space ($z_{0h} + d$ (Oleson *et al.* 2004)) (Vidale & Stöckli 2005). The first two sensible heat fluxes are positive into and the third is positive away from the canopy air space:

$$C_s \frac{\Delta T_s}{\Delta t} = H_g^{n+1} + H_v^{n+1} - H^{n+1} \qquad \text{(Eq. 1a)}$$

where C_s is the canopy air space heat capacity equal to $\rho_{atm} C_p \Delta z$, ρ_{atm} is the density of atmospheric, or moist, air (kg m^{-3}), and C_p is the specific heat capacity of dry air (J kg^{-1} K^{-1}). Δz is the greater of 4 m and the difference between the top and bottom heights of the canopy. If Δz tended to zero, C_s would tend to zero and the prognostic form of Eq. 1a would reduce to the diagnostic expression used in CLM prior to version 4 (Vidale & Stöckli 2005). Eq. 1a′ is shown as a reminder of an assumption that ceases to be true in CLM version 4:

$$\lim_{C_s \to 0} C_s \frac{\Delta T_s}{\Delta t} = 0 \Rightarrow H^{n+1} = H_g^{n+1} + H_v^{n+1} \qquad \text{(Eq. 1a′)}$$

Do not confuse C_s with the variable in Oleson *et al.* (2004) that represents the turbulent transfer coefficient between soil and canopy air.

Starting from Eq. 1a, we carry the $n + 1$ sensible heat flux terms to the LHS, add the corresponding n terms to both sides of the equation, expand all terms, and rearrange the LHS by variable instead of by time step:

$$C_s \frac{\Delta T_s}{\Delta t} + H^{n+1} - H_g^{n+1} - H_v^{n+1} = 0$$

$$C_s \frac{\Delta T_s}{\Delta t} + H^{n+1} - H^n - H_g^{n+1} + H_g^n - H_v^{n+1} + H_v^n = H_v^n + H_g^n - H^n$$

$$\begin{aligned}
&C_s \frac{\Delta T_s}{\Delta t} - \frac{\rho_{atm} C_p}{r_{ah}}\left(\overline{\theta}_{atm}^{n+1} - T_s^{n+1}\right) + \frac{\rho_{atm} C_p}{r_{ah}}\left(\overline{\theta}_{atm}^{n} - T_s^{n}\right) \\
&+ \frac{\rho_{atm} C_p}{r_{ah'}}\left(T_s^{n+1} - T_g^{n+1}\right) - \frac{\rho_{atm} C_p}{r_{ah'}}\left(T_s^{n} - T_g^{n}\right) \\
&+ \rho_{atm} C_p \frac{L+S}{r_b}\left(T_s^{n+1} - T_v^{n+1}\right) - \rho_{atm} C_p \frac{L+S}{r_b}\left(T_s^{n} - T_v^{n}\right) \\
&= -\rho_{atm} C_p \frac{L+S}{r_b}\left(T_s^{n} - T_v^{n}\right) - \frac{\rho_{atm} C_p}{r_{ah'}}\left(T_s^{n} - T_g^{n}\right) + \frac{\rho_{atm} C_p}{r_{ah}}\left(\overline{\theta}_{atm}^{n} - T_s^{n}\right)
\end{aligned} \qquad \text{(Eq. 1b)}$$

$$\begin{aligned}
&\left(\frac{C_s}{\Delta t} + \frac{\rho_{atm} C_p}{r_{ah}} + \rho_{atm} C_p \frac{L+S}{r_b} + \frac{\rho_{atm} C_p}{r_{ah'}}\right)\left(T_s^{n+1} - T_s^{n}\right) - \frac{\rho_{atm} C_p}{r_{ah}}\left(\overline{\theta}_{atm}^{n+1} - \overline{\theta}_{atm}^{n}\right) \\
&- \frac{\rho_{atm} C_p}{r_{ah'}}\left(T_g^{n+1} - T_g^{n}\right) - \rho_{atm} C_p \frac{L+S}{r_b}\left(T_v^{n+1} - T_v^{n}\right) \\
&= -\rho_{atm} C_p \frac{L+S}{r_b}\left(T_s^{n} - T_v^{n}\right) - \frac{\rho_{atm} C_p}{r_{ah'}}\left(T_s^{n} - T_g^{n}\right) + \frac{\rho_{atm} C_p}{r_{ah}}\left(\overline{\theta}_{atm}^{n} - T_s^{n}\right)
\end{aligned}$$

where T_g and T_v are the ground and leaf temperatures (K), $\overline{\theta}_{atm}$ is the potential temperature (K) at the GCM's reference height, L and S are the exposed leaf and stem area index values (m^2 leaf or stem surface m^{-2} ground), r_{ah} is the aerodynamic resistance to sensible heat transfer (s m^{-1}) between CLM's canopy air space and the GCM's reference height, r_b is the leaf boundary layer resistance (s m^{-1}), and r_{ah}' is the aerodynamic resistance to heat transfer (s m^{-1}) between the ground and the canopy air space. Whether in offline or coupled mode, CLM assumes that a dataset will provide or an AGCM will calculate $\overline{\theta}_{atm}^{n+1}$. Therefore, CLM does not calculate $\overline{\theta}_{atm}^{n+1}$ and assumes instead that $\overline{\theta}_{atm}^{n+1} - \overline{\theta}_{atm}^{n} = 0$ to solve the matrix. The corresponding term in Eq. 1b drops out.

T_s, T_g, and $\overline{\theta}_{atm}$, are column level, while T_v, C_s, and the resistance terms are plant functional type (pft) level variables. Generalizing Eq. 1b to include multiple pfts per column and substituting C_s with $\rho_{atm} C_p \Delta z$ gives:

$$\begin{aligned}
&\sum_{j=1}^{npft}\left[(wt)_j\left(\frac{\Delta z_j}{\Delta t}+\frac{1}{(r_{ah})_j}+\frac{L_j+S_j}{(r_b)_j}+\frac{1}{(r_{ah'})_j}\right)\rho_{atm}C_p\right]\left(T_s^{n+1}-T_s^n\right)\\
&-\sum_{j=1}^{npft}\left[(wt)_j\frac{\rho_{atm}C_p}{(r_{ah'})_j}\right]\left(T_g^{n+1}-T_g^n\right)\\
&-\sum_{j=1}^{npft}\left[(wt)_j\frac{L_j+S_j}{(r_b)_j}\rho_{atm}C_p\left[(T_v^{n+1})_j-(T_v^n)_j\right]\right]\\
&=\sum_{j=1}^{npft}\left[(wt)_j\left(\begin{array}{l}-\rho_{atm}C_p\dfrac{L_j+S_j}{(r_b)_j}\left(T_s^n-(T_v^n)_j\right)\\[2ex]-\dfrac{\rho_{atm}C_p}{(r_{ah'})_j}\left(T_s^n-T_g^n\right)+\dfrac{\rho_{atm}C_p}{(r_{ah})_j}\left(\overline{\theta}_{atm}^n-T_s^n\right)\end{array}\right)\right]
\end{aligned} \qquad \text{(Eq. 1b}'\text{)}$$

where j is the pft index ranging from 1 to $npft$ (the number of pfts present in the column) and $(wt)_j$ is the fraction of the column occupied by pft j, where $\sum_{j=1}^{npft}(wt)_j = 1$. CLM includes bare ground in the same column as the vegetation and gives it a pft index. The fraction of the column with bare ground has $L_j + S_j = 0$.

In matrix coefficient form, Eq. 1b′ becomes:

$$C_{T_s}^1 = \sum_{j=1}^{npft}\left[(wt)_j\left(\frac{\Delta z_j}{2\Delta t} + \frac{1}{(r_{ah})_j} + \frac{L_j + S_j}{(r_b)_j} + \frac{1}{(r_{ah'})_j}\right)\rho_{atm}C_p\right]$$

$$C_{(T_v)_j}^1 = -(wt)_j \frac{L_j + S_j}{(r_b)_j}\rho_{atm}C_p \quad \text{for} \quad j = 1,2,\ldots,npft$$

$$C_{T_g}^1 = -\sum_{j=1}^{npft}\left[(wt)_j \frac{\rho_{atm}C_p}{(r_{ah'})_j}\right] \qquad \text{(Eq. 1c)}$$

$$F_{T_s} = \sum_{j=1}^{npft}\left[(wt)_j\left(\begin{array}{l} -\rho_{atm}C_p \dfrac{L_j + S_j}{(r_b)_j}\left(T_s^n - (T_v^n)_j\right) \\ -\dfrac{\rho_{atm}C_p}{(r_{ah'})_j}\left(T_s^n - T_g^n\right) + \dfrac{\rho_{atm}C_p}{(r_{ah})_j}\left(\overline{\theta}_{atm}^n - T_s^n\right)\end{array}\right)\right]$$

where $C_{T_s}^1$ is the matrix coefficient in row 1 that is multiplied by ΔT_s, $C_{(T_v)_j}^1$ is multiplied by $\Delta(T_v)_j$, and $C_{T_g}^1$ is multiplied by ΔT_g. A smoothing filter is introduced by multiplying the time step, Δt, by a factor of 2. F_{T_s} is the RHS term of Eq. 1.

2.2 Solving for q_s

Eq. 2 solves for q_s, the specific humidity (kg water vapor kg^{-1} air) of the canopy air space. Eq. 2 states that the change in q_s with respect to time is directly proportional to the sum of latent heat fluxes (W m^{-2}) from the ground, λE_g, the vegetation, λE_v, and the GCM's reference height ($z_{atm,w} = z_{atm,h}$ (Oleson *et al.* 2004)), λE, to the canopy air space height (z_{0w} + d = z_{0h} + d (Oleson *et al.* 2004)) (Vidale & Stöckli 2005). The first two latent heat fluxes are positive into and the third is positive away from the canopy air space:

$$\rho_{atm}\lambda\Delta z\frac{\Delta q_s}{\Delta t}=\lambda E_g^{n+1}+\lambda E_v^{n+1}-\lambda E^{n+1} \qquad \text{(Eq. 2a)}$$

where λE_v = λE_v^t + λE_v^w, i.e. the sum of transpiration and canopy evaporation, and λ (J kg^{-1}) is the latent heat of sublimation if the water content of the top soil/snow layer is all ice and no liquid; λ is the latent heat of vaporization when liquid water is present in the soil or when calculating plant *evapo?*transpiration. Without the factor λ, the units of Eq. 2a would have been water vapor flux units (kg m^{-2} s^{-1}) instead of energy flux units (W m^{-2}). Other terms in Eq. 2a have been defined previously.

If Δz tended to zero, the prognostic form of Eq. 2a would reduce to the diagnostic expression used in CLM prior to version 4 (not shown but, e.g., see Eq. 1a′ in section 2.1).

Next we carry the n + 1 latent heat flux terms to the LHS, add the corresponding n terms to both sides of the equation, expand all terms, and rearrange by variable instead of by time step:

$$\rho_{atm}\lambda\Delta z\frac{\Delta q_s}{\Delta t}+\lambda E^{n+1}-\lambda E_g^{n+1}-\lambda E_v^{n+1}=0$$

$$\rho_{atm}\lambda\Delta z\frac{\Delta q_s}{\Delta t}+\lambda E^{n+1}-\lambda E^{n}-\lambda E_g^{n+1}+\lambda E_g^{n}-\lambda E_v^{n+1}+\lambda E_v^{n}=\lambda E_v^{n}+\lambda E_g^{n}-\lambda E^{n}$$

$$\rho_{atm}\lambda\Delta z\frac{\Delta q_s}{\Delta t}-\frac{\rho_{atm}\lambda}{r_{aw}}\left(q_{atm}^{n+1}-q_s^{n+1}\right)+\frac{\rho_{atm}\lambda}{r_{aw}}\left(q_{atm}^{n}-q_s^{n}\right)+\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^{n+1}-q_g^{n+1}\right)-\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^{n}-q_g^{n}\right)$$
$$+\rho_{atm}\lambda\left\{f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right\}\left(q_s^{n+1}-q_{sat}^{T_v^{n+1}}\right)$$
$$-\rho_{atm}\lambda\left\{f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right\}\left(q_s^{n}-q_{sat}^{T_v^{n}}\right)$$
$$=-\rho_{atm}\lambda\left\{f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right\}\left(q_s^{n}-q_{sat}^{T_v^{n}}\right)$$
$$-\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^{n}-q_g^{n}\right)+\frac{\rho_{atm}\lambda}{r_{aw}}\left(q_{atm}^{n}-q_s^{n}\right)$$

$$\rho_{atm}\lambda\left\{\frac{\Delta z}{\Delta t}+\frac{1}{r_{aw}}+f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)+\frac{1}{r_{aw'}}\right\}\left(q_s^{n+1}-q_s^{n}\right)$$
$$-\rho_{atm}\lambda\left\{f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right\}\left(q_{sat}^{T_v^{n+1}}-q_{sat}^{T_v^{n}}\right)$$
$$-\frac{\rho_{atm}\lambda}{r_{aw}}\left(q_{atm}^{n+1}-q_{atm}^{n}\right)-\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_g^{n+1}-q_g^{n}\right) \qquad \text{(Eq. 2b)}$$
$$=-\rho_{atm}\lambda\left\{f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right\}\left(q_s^{n}-q_{sat}^{T_v^{n}}\right)$$
$$-\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^{n}-q_g^{n}\right)+\frac{\rho_{atm}\lambda}{r_{aw}}\left(q_{atm}^{n}-q_s^{n}\right)$$

where f_{wet} is the wetted fraction of the canopy (leaves and stems) and f_{dry} is the fraction of leaves that are dry and able to photosynthesize (f_{wet} and f_{dry} are defined mathematically in Oleson *et al.* (2004) and $f_{dry} \neq 1 - f_{wet}$ in general). When the soil moisture function that limits transpiration $\beta_t \leq 1 \times 10^{-10}$, $f_{dry} = 0$. When dew is present, $f_{dry} = 0$ and $f_{wet} = 1$. L^{sun} and L^{sha} are the parts of L ($m^2\ m^{-2}$) that are sunlit and shaded, r_s^{sun} and r_s^{sha} are the sunlit and shaded stomatal resistances ($s\ m^{-1}$), r_{aw} is the aerodynamic resistance to water vapor transfer ($s\ m^{-1}$) between the canopy air space and the GCM's reference height, r_{aw}' is the aerodynamic resistance to water vapor transfer ($s\ m^{-1}$) between the ground and the canopy air space, q_g is the specific humidity (kg kg^{-1}) at the ground, and $q_{sat}^{T_v}$ is the saturated specific humidity (kg kg^{-1}) at temperature T_v. Whether in offline or coupled mode, CLM assumes that a dataset will provide or an AGCM will calculate q_{atm}^{n+1}. Therefore, CLM does not calculate q_{atm}^{n+1} and assumes instead that $q_{atm}^{n+1} - q_{atm}^{n} = 0$ to solve the matrix. The corresponding term in Eq. 2b drops out.

Assuming that $\frac{dq_{sat}^{T}}{dT} = \frac{q_{sat}^{T^{n+1}} - q_{sat}^{T^{n}}}{T^{n+1} - T^{n}}$, where q_{sat}^{T} is the saturated specific humidity at temperature T, and assuming that $q_g = \alpha q_{sat}^{T_g}$, where q_g is the specific humidity at the ground as a function of the saturated specific humidity at the ground (section 5.2 of Oleson et al. (2004)), we substitute the terms $q_g^{n+1} - q_g^{n}$ and $q_{sat}^{T_v^{n+1}} - q_{sat}^{T_v^{n}}$ to get Eq. 2b′:

$$
\begin{aligned}
&\rho_{atm}\lambda\left\{\frac{\Delta z}{\Delta t} + \frac{1}{r_{aw}} + f_{wet}\frac{L+S}{r_b} + \frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b + r_s^{sun}} + \frac{L^{sha}}{r_b + r_s^{sha}}\right) + \frac{1}{r_{aw'}}\right\}\left(q_s^{n+1} - q_s^{n}\right) \\
&-\rho_{atm}\lambda\frac{dq_{sat}^{T_v}}{dT_v}\left\{f_{wet}\frac{L+S}{r_b} + \frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b + r_s^{sun}} + \frac{L^{sha}}{r_b + r_s^{sha}}\right)\right\}\left(T_v^{n+1} - T_v^{n}\right) \\
&-\frac{\rho_{atm}\lambda}{r_{aw'}}\frac{dq_g}{dT_g}\left(T_g^{n+1} - T_g^{n}\right) \qquad \text{(Eq. 2b′)} \\
&= -\rho_{atm}\lambda\left\{f_{wet}\frac{L+S}{r_b} + \frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b + r_s^{sun}} + \frac{L^{sha}}{r_b + r_s^{sha}}\right)\right\}\left(q_s^{n} - q_{sat}^{T_v^{n}}\right) \\
&-\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^{n} - q_g^{n}\right) + \frac{\rho_{atm}\lambda}{r_{aw}}\left(q_{atm}^{n} - q_s^{n}\right)
\end{aligned}
$$

T_g, q_s, and q_{atm}, are column level, while T_v and the resistance terms are pft level variables. Generalizing Eq. 2b′ to include multiple pfts per column gives:

$$
\sum_{j=1}^{npft}\left[(wt)_j\,\rho_{atm}\lambda\left\{\begin{array}{l}\dfrac{\Delta z_j}{\Delta t}+\dfrac{1}{(r_{aw})_j}+\dfrac{1}{(r_{aw'})_j}+(f_{wet})_j\,\dfrac{L_j+S_j}{(r_b)_j}\\ +\dfrac{(f_{dry})_j}{L_j}\left(\dfrac{L_j^{sun}}{(r_b)_j+(r_s^{sun})_j}+\dfrac{L_j^{sha}}{(r_b)_j+(r_s^{sha})_j}\right)\end{array}\right\}\right]\left(q_s^{n+1}-q_s^{n}\right)
$$

$$
-\sum_{j=1}^{npft}\left[(wt)_j\,\rho_{atm}\lambda\,\frac{dq_{sat}^{(T_v)_j}}{d(T_v)_j}\left\{\begin{array}{l}(f_{wet})_j\,\dfrac{L_j+S_j}{(r_b)_j}\\ +\dfrac{(f_{dry})_j}{L_j}\left(\dfrac{L_j^{sun}}{(r_b)_j+(r_s^{sun})_j}+\dfrac{L_j^{sha}}{(r_b)_j+(r_s^{sha})_j}\right)\end{array}\right\}\left[(T_v^{n+1})_j-(T_v^{n})_j\right]\right]
$$

$$
-\sum_{j=1}^{npft}\left[(wt)_j\,\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\frac{dq_g}{dT_g}\right]\left(T_g^{n+1}-T_g^{n}\right) \qquad \text{(Eq.2b")}
$$

$$
=\sum_{j=1}^{npft}\left[(wt)_j\left(\begin{array}{l}-\rho_{atm}\lambda\left\{(f_{wet})_j\,\dfrac{L_j+S_j}{(r_b)_j}+\dfrac{(f_{dry})_j}{L_j}\left(\dfrac{L_j^{sun}}{(r_b)_j+(r_s^{sun})_j}+\dfrac{L_j^{sha}}{(r_b)_j+(r_s^{sha})_j}\right)\right\}\left(q_s^{n}-q_{sat}^{(T_v^n)_j}\right)\\ -\dfrac{\rho_{atm}\lambda}{(r_{aw'})_j}\left(q_s^{n}-q_g^{n}\right)+\dfrac{\rho_{atm}\lambda}{(r_{aw})_j}\left(q_{atm}^{n}-q_s^{n}\right)\end{array}\right)\right]
$$

In matrix coefficient form, Eq. 2b″ becomes:

$$
C_{q_s}^2=\sum_{j=1}^{npft}\left[(wt)_j\,\rho_{atm}\lambda\left\{\begin{array}{l}\dfrac{\Delta z_j}{2\Delta t}+\dfrac{1}{(r_{aw})_j}+\dfrac{1}{(r_{aw'})_j}+(f_{wet})_j\,\dfrac{L_j+S_j}{(r_b)_j}\\ +\dfrac{(f_{dry})_j}{L_j}\left(\dfrac{L_j^{sun}}{(r_b)_j+(r_s^{sun})_j}+\dfrac{L_j^{sha}}{(r_b)_j+(r_s^{sha})_j}\right)\end{array}\right\}\right]
$$

$$
C_{(T_v)_j}^2=-(wt)_j\,\rho_{atm}\lambda\,\frac{dq_{sat}^{(T_v)_j}}{d(T_v)_j}\left\{\begin{array}{l}(f_{wet})_j\,\dfrac{L_j+S_j}{(r_b)_j}\\ +\dfrac{(f_{dry})_j}{L_j}\left(\dfrac{L_j^{sun}}{(r_b)_j+(r_s^{sun})_j}+\dfrac{L_j^{sha}}{(r_b)+(r_s^{sha})_j}\right)\end{array}\right\}\ \text{for } j=1,2,\ldots,npft
$$

$$
C_{T_g}^2=-\sum_{j=1}^{npft}\left[(wt)_j\,\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\frac{dq_g}{dT_g}\right] \qquad \text{(Eq.2c)}
$$

$$
F_{q_s}=\sum_{j=1}^{npft}\left[(wt)_j\left(\begin{array}{l}-\rho_{atm}\lambda\left\{(f_{wet})_j\,\dfrac{L_j+S_j}{(r_b)_j}+\dfrac{(f_{dry})_j}{L_j}\left(\dfrac{L_j^{sun}}{(r_b)_j+(r_s^{sun})_j}+\dfrac{L_j^{sha}}{(r_b)_j+(r_s^{sha})_j}\right)\right\}\left(q_s^{n}-q_{sat}^{(T_v^n)_j}\right)\\ -\dfrac{\rho_{atm}\lambda}{(r_{aw'})_j}\left(q_s^{n}-q_g^{n}\right)+\dfrac{\rho_{atm}\lambda}{(r_{aw})_j}\left(q_{atm}^{n}-q_s^{n}\right)\end{array}\right)\right]
$$

where $C^2_{q_s}$ is the matrix coefficient in row 2 that is multiplied by Δq_s, $C^2_{(T_v)_j}$ is multiplied by $\Delta(T_v)_j$, and $C^2_{T_g}$ is multiplied by ΔT_g. A smoothing filter is introduced by multiplying the time step, Δt, by a factor of 2. F_{q_s} is the RHS term of Eq. 2. Although λ could cancel out of all the terms in Eq. 2 as latent heat of vaporization, λ could also represent the latent heat of sublimation in $C^2_{T_g}$ if the top soil/snow layer's moisture is all ice. Therefore, we keep λ in all the terms of Eq. 2.

2.3 Solving for T_v (We'll solve separately for sunlit and shaded leaf temperatures later.)

Eq. 3 states that vegetation temperature, T_v (K), changes with time as a function of the net energy available to the vegetation (W m^{-2}), accounting for radiation and heat flux terms, as well as changes in emitted longwave radiation from the ground and vegetation. The radiation terms include the vegetation-absorbed net solar, $\vec{S}_v$ (positive into vegetation), and net longwave radiation, $\vec{L}_v$ (positive away from vegetation). The heat flux terms include the sensible and latent heat fluxes, H_v and λE_v (positive away from vegetation). The changes in longwave radiation emitted by the ground and vegetation for respective temperature changes ΔT_g and ΔT_v from time step n to n + 1, are given by $\left.\frac{dL_g \uparrow}{dT_g}\right|_n \Delta T_g \delta_{veg}$ (positive into vegetation) and $\left.\frac{dL_v \updownarrow}{dT_v}\right|_n \Delta T_v \delta_{veg}$ (positive away from vegetation). *Feels as though we are neglecting other longwave terms like the above.*

$$C_v \frac{\Delta T_v}{\Delta t} = \vec{S}_v^n - \vec{L}_v^n - H_v^{n+1} - \lambda E_v^{n+1} + \left.\frac{dL_g \uparrow}{dT_g}\right|_n \Delta T_g \delta_{veg} - \left.\frac{dL_v \updownarrow}{dT_v}\right|_n \Delta T_v \delta_{veg} \qquad \text{(Eq. 3a)}$$

where C_v (J m^{-2} K^{-1}) is the heat capacity of the vegetation equal to $(L+S)C_{liq}W_{leaf} + C_{liq}W_{can}$, where C_{liq} is the specific heat capacity of water (J kg^{-1} K^{-1}), W_{leaf} is the amount of water in leaves per leaf area set to 0.2 kg m^{-2} (does Ian mean in leaves+stems per leaf+stem area?), W_{can} is the amount of water on the canopy per unit area of ground (kg m^{-2}), and δ_{veg} is a step function equal to zero for $L + S < 0.05$ and equal to one otherwise.

As in previous sections, now we transform Eq. 3a to Eq. 3b. Also we replace $\left.\frac{dL_g \uparrow}{dT_g}\right|_n$ and $\left.\frac{dL_v \updownarrow}{dT_v}\right|_n$ with $4\varepsilon_g \sigma \left(T_g^n\right)^3$ and $2 \cdot 4\varepsilon_v \sigma \left(T_v^n\right)^3$ respectively:

$$C_v \frac{\Delta T_v}{\Delta t} + H_v^{n+1} - H_v^n + \lambda E_v^{n+1} - \lambda E_v^n + \left.\frac{dL_v \updownarrow}{dT_v}\right|_n \Delta T_v - \left.\frac{dL_g \uparrow}{dT_g}\right|_n \Delta T_g = \vec{S}_v^n - \vec{L}_v^n - H_v^n - \lambda E_v^n$$

$$\begin{aligned}
&\frac{C_v}{\Delta t}\left(T_v^{n+1} - T_v^n\right) - \rho_{atm} C_p \frac{L+S}{r_b}\left(T_s^{n+1} - T_v^{n+1}\right) + \rho_{atm} C_p \frac{L+S}{r_b}\left(T_s^n - T_v^n\right) \\
&- \rho_{atm}\lambda \left[f_{wet}\frac{L+S}{r_b} + \frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b + r_s^{sun}} + \frac{L^{sha}}{r_b + r_s^{sha}} \right) \right]\left(q_s^{n+1} - q_{sat}^{T_v^{n+1}}\right) \\
&+ \rho_{atm}\lambda \left[f_{wet}\frac{L+S}{r_b} + \frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b + r_s^{sun}} + \frac{L^{sha}}{r_b + r_s^{sha}} \right) \right]\left(q_s^{n} - q_{sat}^{T_v^{n}}\right) \\
&+ 8\varepsilon_v \sigma \left(T_v^n\right)^3 \delta_{veg}\left(T_v^{n+1} - T_v^n\right) - 4\varepsilon_g \sigma \left(T_g^n\right)^3 \delta_{veg}\left(T_g^{n+1} - T_g^n\right) \\
&= \vec{S}_v^n - \vec{L}_v^n + \rho_{atm} C_p \frac{L+S}{r_b}\left(T_s^n - T_v^n\right) + \rho_{atm}\lambda \left[f_{wet}\frac{L+S}{r_b} + \frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b + r_s^{sun}} + \frac{L^{sha}}{r_b + r_s^{sha}} \right) \right]\left(q_s^{n} - q_{sat}^{T_v^{n}}\right)
\end{aligned}$$

$$
\begin{aligned}
&\left[\frac{C_v}{\Delta t}+8\varepsilon_v\sigma\left(T_v^n\right)^3\delta_{veg}+\rho_{atm}C_p\frac{L+S}{r_b}\right]\left(T_v^{n+1}-T_v^n\right)-\rho_{atm}C_p\frac{L+S}{r_b}\left(T_s^{n+1}-T_s^n\right)\\
&+\rho_{atm}\lambda\left[f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right]\left(q_{sat}^{T_v^{n+1}}-q_{sat}^{T_v^n}\right)\\
&-\rho_{atm}\lambda\left[f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right]\left(q_s^{n+1}-q_s^n\right)\\
&-4\varepsilon_g\sigma\left(T_g^n\right)^3\delta_{veg}\left(T_g^{n+1}-T_g^n\right)\\
&=\vec{S}_v^n-\vec{L}_v^n+\rho_{atm}C_p\frac{L+S}{r_b}\left(T_s^n-T_v^n\right)+\rho_{atm}\lambda\left[f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right]\left(q_s^n-q_{sat}^{T_v^n}\right)
\end{aligned}
\qquad \text{(Eq. 3b)}
$$

where ε_v and ε_g are the vegetation and ground emissivities, and σ is the Stefan-Boltzmann constant (W m^{-2} K^{-4}).

As done in Eq. 2b, we next substitute $q_{sat}^{T_v^{n+1}}-q_{sat}^{T_v^n}$ with $\frac{dq_{sat}^{T_v}}{dT_v}\left(T_v^{n+1}-T_v^n\right)$:

$$
\begin{aligned}
&\left[\frac{C_v}{\Delta t}+8\varepsilon_v\sigma\left(T_v^n\right)^3\delta_{veg}+\rho_{atm}C_p\frac{L+S}{r_b}\right.\\
&\left.+\rho_{atm}\lambda\frac{dq_{sat}^{T_v}}{dT_v}\left\{f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right\}\right]\left(T_v^{n+1}-T_v^n\right)\\
&-\rho_{atm}\lambda\left[f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right]\left(q_s^{n+1}-q_s^n\right)\\
&-\rho_{atm}C_p\frac{L+S}{r_b}\left(T_s^{n+1}-T_s^n\right)-4\varepsilon_g\sigma\left(T_g^n\right)^3\delta_{veg}\left(T_g^{n+1}-T_g^n\right)\\
&=\vec{S}_v^n-\vec{L}_v^n+\rho_{atm}C_p\frac{L+S}{r_b}\left(T_s^n-T_v^n\right)+\rho_{atm}\lambda\left[f_{wet}\frac{L+S}{r_b}+\frac{f_{dry}}{L}\left(\frac{L^{sun}}{r_b+r_s^{sun}}+\frac{L^{sha}}{r_b+r_s^{sha}}\right)\right]\left(q_s^n-q_{sat}^{T_v^n}\right)
\end{aligned}
\qquad \text{(Eq. 3b')}
$$

T_s, q_s, and T_g are column level, while T_v and the resistance terms are pft level variables. Generalizing Eq. 3b′ to include multiple pfts per column gives:

$$\left[\frac{(C_v)_j}{\Delta t} + 8(\varepsilon_v)_j \sigma\left(T_v^n\right)_j^3 (\delta_{veg})_j + \rho_{atm} C_p \frac{L_j + S_j}{(r_b)_j}\right.$$

$$\left.+ \rho_{atm} \lambda \frac{dq_{sat}^{(T_v)_j}}{d(T_v)_j}\left\{(f_{wet})_j \frac{L_j + S_j}{(r_b)_j} + \frac{(f_{dry})_j}{L_j}\left(\frac{L_j^{sun}}{(r_b)_j + (r_s^{sun})_j} + \frac{L_j^{sha}}{(r_b)_j + (r_s^{sha})_j}\right)\right\}\right]\left[(T_v^{n+1})_j - (T_v^n)_j\right]$$

$$- \rho_{atm} \lambda \left[(f_{wet})_j \frac{L_j + S_j}{(r_b)_j} + \frac{(f_{dry})_j}{L_j}\left(\frac{L_j^{sun}}{(r_b)_j + (r_s^{sun})_j} + \frac{L_j^{sha}}{(r_b)_j + (r_s^{sha})_j}\right)\right]\left(q_s^{n+1} - q_s^n\right)$$

$$- \rho_{atm} C_p \frac{L_j + S_j}{(r_b)_j}\left(T_s^{n+1} - T_s^n\right) - 4\varepsilon_g \sigma\left(T_g^n\right)^3 (\delta_{veg})_j \left(T_g^{n+1} - T_g^n\right) \qquad \text{(Eq. 3b'')}$$

$$= (\vec{S}_v^n)_j - (\vec{L}_v^n)_j + \rho_{atm} C_p \frac{L_j + S_j}{(r_b)_j}\left(T_s^n - (T_v^n)_j\right)$$

$$+ \rho_{atm} \lambda \left[(f_{wet})_j \frac{L_j + S_j}{(r_b)_j} + \frac{(f_{dry})_j}{L_j}\left(\frac{L_j^{sun}}{(r_b)_j + (r_s^{sun})_j} + \frac{L_j^{sha}}{(r_b)_j + (r_s^{sha})_j}\right)\right]\left(q_s^n - q_{sat}^{(T_v^n)_j}\right)$$

for j = 1, 2, …, *npft*. There are as many equations solving for T_v as pfts in the column.

In matrix coefficient form, Eq. 3b″ becomes:

$$C_{T_s}^{2+j} = -\rho_{atm} C_p \frac{L_j + S_j}{(r_b)_j}$$

$$C_{q_s}^{2+j} = -\rho_{atm} \lambda \left\{(f_{wet})_j \frac{L_j + S_j}{(r_b)_j} + \frac{(f_{dry})_j}{L_j}\left(\frac{L_j^{sun}}{(r_b)_j + (r_s^{sun})_j} + \frac{L_j^{sha}}{(r_b)_j + (r_s^{sha})_j}\right)\right\}$$

$$C_{(T_v)_j}^{2+j} = \frac{(C_v)_j}{2\Delta t} + 8(\varepsilon_v)_j \sigma\left(T_v^n\right)_j^3 (\delta_{veg})_j + \rho_{atm} C_p \frac{L_j + S_j}{(r_b)_j} \qquad \text{(Eq. 3c)}$$

$$+ \rho_{atm} \lambda \frac{dq_{sat}^{(T_v)_j}}{d(T_v)_j}\left\{(f_{wet})_j \frac{L_j + S_j}{(r_b)_j} + \frac{(f_{dry})_j}{L_j}\left(\frac{L_j^{sun}}{(r_b)_j + (r_s^{sun})_j} + \frac{L_j^{sha}}{(r_b)_j + (r_s^{sha})_j}\right)\right\}$$

$$C_{T_g}^{2+j} = -4\varepsilon_g \sigma\left(T_g^n\right)^3 (\delta_{veg})_j$$

$$F_{(T_v)_j}\Big|_{j=1}^{npft} = (\vec{S}_v^n)_j - (\vec{L}_v^n)_j + \rho_{atm} C_p \frac{L_j + S_j}{(r_b)_j}\left(T_s^n - (T_v^n)_j\right)$$

$$+ \rho_{atm} \lambda \left[(f_{wet})_j \frac{L_j + S_j}{(r_b)_j} + \frac{(f_{dry})_j}{L_j}\left(\frac{L_j^{sun}}{(r_b)_j + (r_s^{sun})_j} + \frac{L_j^{sha}}{(r_b)_j + (r_s^{sha})_j}\right)\right]\left(q_s^n - q_{sat}^{(T_v^n)_j}\right)$$

for j = 1, 2, …, *npft*. $C_{T_s}^{2+j}$ is the matrix coefficient in row 2 + j that is multiplied by ΔT_s, $C_{q_s}^{2+j}$ is multiplied by Δq_s, $C_{(T_v)_j}^{2+j}$ is multiplied by $\Delta (T_v)_j$, and $C_{T_g}^{2+j}$ is multiplied by ΔT_g. A smoothing filter is introduced by multiplying the time step, Δt, by a factor of 2. $F_{(T_v)_j}$ is the RHS term of Eq. 3.

The matrix solves for $(T_v)_j$ for all the pfts present in a column. For simplicity we continue section 2 as though *npft* equals one. Therefore, this section (2.3) discussed matrix row 3, the following section (2.4) will discuss matrix row 4, and so on.

2.4 Solving for T_g

In CLM, properties of the ground correspond to properties of the top soil or snow layer, whichever is in contact with the atmosphere. Eq. 4 solves for T_g, the ground temperature (K), stating that $\frac{\Delta T_g}{\Delta t}$ is a function of the net energy available to the top soil/snow layer (W m^{-2}). As in section 2.3, net energy includes radiation and heat flux terms, as well as the changes in longwave radiation emitted by the ground and vegetation. The radiation terms include ground-absorbed net solar, $\vec{S}_g$ (positive into the top soil/snow layer), and net longwave radiation, $\vec{L}_g$ (positive away from top soil/snow layer). The heat flux terms include sensible, latent, and soil heat fluxes, H_g, λE_g, and F_{1+snl} (positive away from top soil/snow layer). The changes in longwave radiation emitted by the ground and vegetation for respective temperature changes ΔT_g and ΔT_v

from time step n to $n + 1$, are given by $\left.\frac{dL_g \uparrow}{dT_g}\right|_n \Delta T_g$ (positive away from top soil/snow layer) and $\left.\frac{dL_v \downarrow}{dT_v}\right|_n \Delta T_v \delta_{veg}$ (positive into top soil/snow layer):

$$c_{1+snl} \Delta z_{1+snl} \frac{\Delta T_g}{\Delta t} = \vec{S}_g^n - \vec{L}_g^n - H_g^{n+1} - \lambda E_g^{n+1} - F_{1+snl}^{n+1} - \left.\frac{dL_g \uparrow}{dT_g}\right|_n \Delta T_g + \left.\frac{dL_v \downarrow}{dT_v}\right|_n \Delta T_v \delta_{veg} \text{ (Eq. 4a)}$$

where c_{1+snl} (J m^{-3} K^{-1}) is the volumetric heat capacity of the top soil/snow layer (index 1+*snl*) and *snl*, the number of snow layers, can range from 0 to –5. With no snow the index for the top soil layer is 1, while with five layers of snow the index for the top snow layer is –4. Δz_{1+snl} (m) is the top soil/snow layer thickness.

Transformations similar to the ones used in sections 2.2 and 2.3 lead from Eq. 4a to Eq. 4b. $\left.\frac{dL_g \uparrow}{dT_g}\right|_n$ and $\left.\frac{dL_v \downarrow}{dT_v}\right|_n$ are replaced with $4\varepsilon_g \sigma \left(T_g^n\right)^3$ and $4\varepsilon_v \sigma \left(T_v^n\right)^3$ respectively, and $q_g^{n+1} - q_g^n$ is replaced with $\frac{dq_g}{dT_g}\left(T_g^{n+1} - T_g^n\right)$:

$$c_{1+snl} \Delta z_{1+snl} \frac{\Delta T_g}{\Delta t} + \left.\frac{dL_g \uparrow}{dT_g}\right|_n \Delta T_g - \left.\frac{dL_v \downarrow}{dT_v}\right|_n \Delta T_v \delta_{veg}$$
$$+ H_g^{n+1} - H_g^n + \lambda E_g^{n+1} - \lambda E_g^n + F_{1+snl}^{n+1} - F_{1+snl}^n = \vec{S}_g^n - \vec{L}_g^n - H_g^n - \lambda E_g^n - F_{1+snl}^n$$

$$c_{1+snl} \Delta z_{1+snl} \frac{\Delta T_g}{\Delta t} + 4\varepsilon_g \sigma \left(T_g^n\right)^3 \left(T_g^{n+1} - T_g^n\right) - 4\varepsilon_v \sigma \left(T_v^n\right)^3 \delta_{veg} \left(T_v^{n+1} - T_v^n\right)$$
$$- \frac{\rho_{atm} C_p}{r_{ah'}} \left(T_s^{n+1} - T_g^{n+1}\right) + \frac{\rho_{atm} C_p}{r_{ah'}} \left(T_s^n - T_g^n\right) - \frac{\rho_{atm} \lambda}{r_{aw'}} \left(q_s^{n+1} - q_g^{n+1}\right) + \frac{\rho_{atm} \lambda}{r_{aw'}} \left(q_s^n - q_g^n\right)$$
$$- \frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl} - z_{1+snl}} \left(T_g^{n+1} - T_{2+snl}^{n+1}\right) + \frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl} - z_{1+snl}} \left(T_g^n - T_{2+snl}^n\right)$$
$$= \vec{S}_g^n - \vec{L}_g^n + \frac{\rho_{atm} C_p}{r_{ah'}} \left(T_s^n - T_g^n\right) + \frac{\rho_{atm} \lambda}{r_{aw'}} \left(q_s^n - q_g^n\right) + \frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl} - z_{1+snl}} \left(T_g^n - T_{2+snl}^n\right)$$

$$
\begin{aligned}
& c_{1+snl}\Delta z_{1+snl}\frac{\Delta T_g}{\Delta t}+\left[\frac{\rho_{atm}C_p}{r_{ah'}}+4\varepsilon_g\sigma\left(T_g^n\right)^3-\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\right]\left(T_g^{n+1}-T_g^n\right) \\
& -\frac{\rho_{atm}C_p}{r_{ah'}}\left(T_s^{n+1}-T_s^n\right)-\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^{n+1}-q_s^n\right)+\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_g^{n+1}-q_g^n\right) \\
& +\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\left(T_{2+snl}^{n+1}-T_{2+snl}^n\right)-4\varepsilon_v\sigma\left(T_v^n\right)^3\delta_{veg}\left(T_v^{n+1}-T_v^n\right) \\
& =\vec{S}_g^n-\vec{L}_g^n+\frac{\rho_{atm}C_p}{r_{ah'}}\left(T_s^n-T_g^n\right)+\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^n-q_g^n\right)+\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\left(T_g^n-T_{2+snl}^n\right)
\end{aligned}
\qquad \text{(Eq. 4b)}
$$

$$
\begin{aligned}
& \left[\frac{c_{1+snl}\Delta z_{1+snl}}{\Delta t}+\frac{\rho_{atm}C_p}{r_{ah'}}+\frac{\rho_{atm}\lambda}{r_{aw'}}\frac{dq_g}{dT_g}+4\varepsilon_g\sigma\left(T_g^n\right)^3-\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\right]\left(T_g^{n+1}-T_g^n\right) \\
& +\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\left(T_{2+snl}^{n+1}-T_{2+snl}^n\right)-4\varepsilon_v\sigma\left(T_v^n\right)^3\delta_{veg}\left(T_v^{n+1}-T_v^n\right) \\
& -\frac{\rho_{atm}C_p}{r_{ah'}}\left(T_s^{n+1}-T_s^n\right)-\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^{n+1}-q_s^n\right) \\
& =\vec{S}_g^n-\vec{L}_g^n+\frac{\rho_{atm}C_p}{r_{ah'}}\left(T_s^n-T_g^n\right)+\frac{\rho_{atm}\lambda}{r_{aw'}}\left(q_s^n-q_g^n\right)+\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\left(T_g^n-T_{2+snl}^n\right)
\end{aligned}
$$

where the coefficient λ was defined in section 2.2, while $\lambda[z_{h,1+snl}]$ (W m^{-1} K^{-1}) is the thermal conductivity at the interface between the top and second soil/snow layers, $z_{h,1+snl}$ (m) refers to the depth of that interface, while z_{1+snl} and z_{2+snl} (m) are the depths of the top and second from the top soil/snow layers, respectively.

T_s, q_s, T_g and T_{2+snl} are column level, while T_v and the resistance terms are pft level variables. Generalizing Eq. 4b for multiple pfts per column gives:

$$\sum_{j=1}^{npft}\left[(wt)_j\left\{\frac{c_{1+snl}\Delta z_{1+snl}}{\Delta t}+\frac{\rho_{atm}C_p}{(r_{ah'})_j}+\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\frac{dq_g}{dT_g}+4\varepsilon_g\sigma\left(T_g^n\right)^3-\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\right\}\right]\left(T_g^{n+1}-T_g^n\right)$$

$$+\sum_{j=1}^{npft}\left[(wt)_j\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\right]\left(T_{2+snl}^{n+1}-T_{2+snl}^n\right)$$

$$-\sum_{j=1}^{npft}\left[(wt)_j 4\varepsilon_v\sigma\left(T_v^n\right)_j^3(\delta_{veg})_j\left[(T_v^{n+1})_j-(T_v^n)_j\right]\right]$$

$$-\sum_{j=1}^{npft}\left[(wt)_j\frac{\rho_{atm}C_p}{(r_{ah'})_j}\right]\left(T_s^{n+1}-T_s^n\right)-\sum_{j=1}^{npft}\left[(wt)_j\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\right]\left(q_s^{n+1}-q_s^n\right) \qquad \text{(Eq. 4b}'\text{)}$$

$$=\sum_{j=1}^{npft}\left[(wt)_j\left(\begin{array}{l}\vec{S}_g^n-\vec{L}_g^n+\frac{\rho_{atm}C_p}{(r_{ah'})_j}\left(T_s^n-T_g^n\right)+\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\left(q_s^n-q_g^n\right)\\+\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\left(T_g^n-T_{2+snl}^n\right)\end{array}\right)\right]$$

In matrix coefficient form, Eq. 4b′ becomes:

$$C_{T_s}^4=-\sum_{j=1}^{npft}\left[(wt)_j\frac{\rho_{atm}C_p}{(r_{ah'})_j}\right]$$

$$C_{q_s}^4=-\sum_{j=1}^{npft}\left[(wt)_j\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\right]$$

$$C_{(T_v)_j}^4\Big|_{j=1}^{npft}=-(wt)_j 4\varepsilon_v\sigma\left(T_v^n\right)_j^3(\delta_{veg})_j \quad \text{for} \quad j=1,2,\ldots,npft$$

$$C_{T_g}^4=\sum_{j=1}^{npft}\left[(wt)_j\left\{\frac{c_{1+snl}\Delta z_{1+snl}}{2\Delta t}+\frac{\rho_{atm}C_p}{(r_{ah'})_j}+\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\frac{dq_g}{dT_g}+4\varepsilon_g\sigma\left(T_g^n\right)^3-\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\right\}\right]$$

$$C_{T_{2+snl}}^4=\sum_{j=1}^{npft}\left[(wt)_j\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\right]$$

$$F_{T_g}=\sum_{j=1}^{npft}\left[(wt)_j\left(\begin{array}{l}\vec{S}_g^n-\vec{L}_g^n+\frac{\rho_{atm}C_p}{(r_{ah'})_j}\left(T_s^n-T_g^n\right)+\frac{\rho_{atm}\lambda}{(r_{aw'})_j}\left(q_s^n-q_g^n\right)\\+\frac{\lambda\left[z_{h,1+snl}\right]}{z_{2+snl}-z_{1+snl}}\left(T_g^n-T_{2+snl}^n\right)\end{array}\right)\right] \qquad \text{(Eq. 4c)}$$

where $C_{T_s}^4$ is the matrix coefficient in row 4 that is multiplied by ΔT_s, $C_{q_s}^4$ is multiplied by Δq_s, $C_{(T_v)_j}^4$ is multiplied by $\Delta(T_v)_j$, $C_{T_g}^4$ is multiplied by ΔT_g, and $C_{T_{2+snl}}^4$ is multiplied by ΔT_{2+snl}. A smoothing filter is introduced by multiplying the time step, Δt, by a factor of 2. F_{T_g} is the RHS term of Eq. 4.

2.5 Solving for T_i

Eq. 5 solves for T_i, the temperature (K) of internal soil/snow layers. In CLM the soil/snow layer index, *i*, ranges from 1 to 10 for soil, while for snow it depends on the number of snow layers, *snl*. For *snl* equal to 0, values of *i* for snow do not exist. For the maximum absolute value of $|snl| = |-5|$, *i* ranges from 0 to –4. Eq. 5 solves for internal layers only, where *i* ranges from a minimum of –3 to a maximum of 9, so Eq. 5 can occupy as many as 13 rows and 13 columns in the final matrix of equations (section 3).

The physical form of Eq. 5 states that soil/snow temperature in layer *i* changes with time as a function of the total heat flux (W m^{-2}) at this layer's interfaces. In particular, F_i^{n+1} is the heat flux at time step *n* + 1 at the interface between layers *i* and *i* + 1 and is positive into layer *i*. Similarly, F_{i-1}^{n+1} is the heat flux at time step *n* + 1 at the interface between layers *i – 1* and *i* and is positive away from layer *i*.

$$c_i \Delta z_i \frac{\Delta T_i}{\Delta t} = F_i^{n+1} - F_{i-1}^{n+1} \qquad \text{(Eq. 5a)}$$

where c_i (J m^{-3} K^{-1}) is the volumetric heat capacity and Δz_i (m) the thickness of the soil/snow layer.

Next we carry the *n* + 1 heat flux terms to the LHS, add the corresponding *n* terms to both sides of the equation, expand all terms, and rearrange by variable instead of by time step:

$$
\begin{aligned}
& c_i \Delta z_i \frac{\Delta T_i}{\Delta t} + F_{i-1}^{n+1} - F_{i-1}^{n} - F_i^{n+1} + F_i^{n} = F_i^{n} - F_{i-1}^{n} \\
& c_i \Delta z_i \frac{\Delta T_i}{\Delta t} - \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}}\left(T_{i-1}^{n+1} - T_i^{n+1}\right) + \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}}\left(T_{i-1}^{n} - T_i^{n}\right) \\
& + \frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i}\left(T_i^{n+1} - T_{i+1}^{n+1}\right) - \frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i}\left(T_i^{n} - T_{i+1}^{n}\right) \\
& = -\frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i}\left(T_i^{n} - T_{i+1}^{n}\right) + \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}}\left(T_{i-1}^{n} - T_i^{n}\right) \\
& - \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}}\left(T_{i-1}^{n+1} - T_{i-1}^{n}\right) + \left(\frac{c_i \Delta z_i}{\Delta t} + \frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i} + \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}}\right)\left(T_i^{n+1} - T_i^{n}\right) \\
& - \frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i}\left(T_{i+1}^{n+1} - T_{i+1}^{n}\right) \\
& = -\frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i}\left(T_i^{n} - T_{i+1}^{n}\right) + \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}}\left(T_{i-1}^{n} - T_i^{n}\right)
\end{aligned}
\qquad \text{(Eq. 5b)}
$$

where $\lambda[z_{h,i}]$ (W m^{-1} K^{-1}) is the thermal conductivity at the interface between soil/snow layers i and i + 1, $z_{h,i}$ (m) refers to the depth of that interface, and z_i (m) is the depth of soil/snow layer i.

In matrix coefficient form, Eq. 5b becomes:

$$
\begin{aligned}
C_{T_{i-1}}^{7} &= -\frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}} \\
C_{T_i}^{7} &= \frac{c_i \Delta z_i}{\Delta t} + \frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i} + \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}} \\
C_{T_{i+1}}^{7} &= -\frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i} \\
F_{T_i} &= -\frac{\lambda\left[z_{h,i}\right]}{z_{i+1} - z_i}\left(T_i^{n} - T_{i+1}^{n}\right) + \frac{\lambda\left[z_{h,i-1}\right]}{z_i - z_{i-1}}\left(T_{i-1}^{n} - T_i^{n}\right)
\end{aligned}
\qquad \text{(Eq. 5c)}
$$

where $C_{T_{i-1,i,i+1}}^{5}$ are the matrix coefficients in row 5 multiplied by $\Delta T_{i-1,i,i+1}$. In Eq. 5, i ranges from 2 to 9 when snl = 0 and from –3 to 9 when snl = –5. The 2Δt smoothing filter found in previous equations is not used in Eq. 5. F_{T_i} is the RHS term of Eq. 5.

2.6 Solving for T_N

Eq. 6 solves for T_N, the temperature (K) of the bottom soil layer (index N). N equals 10 by default in CLM. According to Eq. 6, the change in T_N with time is directly proportional to the soil heat flux into soil layer N, F_{N-1} (W m^{-2}):

$$c_N \Delta z_N \frac{\Delta T_N}{\Delta t} = -F_{N-1}^{n+1} \qquad \text{(Eq. 6a)}$$

where c_N (J m^{-3} K^{-1}) is the volumetric heat capacity and Δz_N (m) the thickness of the bottom soil layer.

$$\begin{aligned} & c_N \Delta z_N \frac{\Delta T_N}{\Delta t} + F_{N-1}^{n+1} - F_{N-1}^{n} = -F_{N-1}^{n} \qquad \text{(Eq. 6b)} \\ & c_N \Delta z_N \frac{\Delta T_N}{\Delta t} - \frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}}\left(T_{N-1}^{n+1} - T_N^{n+1}\right) + \frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}}\left(T_{N-1}^{n} - T_N^{n}\right) = \frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}}\left(T_{N-1}^{n} - T_N^{n}\right) \\ & -\frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}}\left(T_{N-1}^{n+1} - T_{N-1}^{n}\right) + \left(\frac{c_N \Delta z_N}{\Delta t} + \frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}}\right)\left(T_N^{n+1} - T_N^{n}\right) = \frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}}\left(T_{N-1}^{n} - T_N^{n}\right) \end{aligned}$$

where $\lambda[z_{h,N-1}]$ (W m^{-1} K^{-1}) is the thermal conductivity at the interface between soil layers N - 1 and N, while $z_{h,N-1}$ (m) refers to the depth of that interface, and z_N and z_{N-1} (m) are the depths of soil layers N and N - 1.

In matrix coefficient form, Eq. 6b becomes:

$$\begin{aligned} C_{T_{N-1}}^{8} &= -\frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}} \\ C_{T_N}^{8} &= \frac{c_N \Delta z_N}{\Delta t} + \frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}} \qquad \text{(Eq. 6c)} \\ F_{T_N} &= \frac{\lambda\left[z_{h,N-1}\right]}{z_N - z_{N-1}}\left(T_{N-1}^{n} - T_N^{n}\right) \end{aligned}$$

where $C^{6}_{T_{N,N-1}}$ are the matrix coefficients in row 6 multiplied by $\Delta T_{N,N-1}$. The $2\Delta t$ smoothing filter found in previous equations is not used in Eq. 6. F_{T_N} is the RHS term of Eq. 6.

3. The Matrix

Using the LAPACK matrix solver DGESV, CLM solves the set of simultaneous equations described in section 2 once per time step *n* for each column in a land grid cell (except over lakes where CLM's existing method remains unchanged). A grid cell's lake, wetland, glacier, urban, and soil fraction each occupies a separate column. The unknowns in this set of equations include various near-surface prognostic temperature and humidity variables for model time step $n + 1$:

The canopy air space temperature and humidity, T_s and q_s, which represent the column's canopy air space state; T_g, the temperature of the top soil/snow layer; T_i, which for $i \le 0$ are snow layer temperatures and for $i > 0$ are soil layer temperatures; $(T_v)_j$, the vegetation temperature indexed by pft *j*, which does not have values over bare ground.

We write the equations in matrix form $(A \cdot x = B)$ for two sample cases. One with only one pft and three snow/soil layers to match the explanations and subsection numbers of section 2, and the other with three of each (pfts, snow layers, and soil layers) as an illustration:

$$
\begin{pmatrix}
C^1_{T_s} & 0 & C^1_{T_v} & C^1_{T_g} & 0 & 0 \\
0 & C^2_{q_s} & C^2_{T_v} & C^2_{T_g} & 0 & 0 \\
C^3_{T_s} & C^3_{q_s} & C^3_{T_v} & C^3_{T_g} & 0 & 0 \\
C^4_{T_s} & C^4_{q_s} & C^4_{T_v} & C^4_{T_g} & C^4_{T_2} & 0 \\
0 & 0 & 0 & C^5_{T_g} & C^5_{T_2} & C^5_{T_3} \\
0 & 0 & 0 & 0 & C^6_{T_2} & C^6_{T_3}
\end{pmatrix}
\times
\begin{bmatrix} \Delta T_s \\ \Delta q_s \\ \Delta T_v \\ \Delta T_g \\ \Delta T_2 \\ \Delta T_3 \end{bmatrix}
=
\begin{bmatrix} F_{T_s} \\ F_{q_s} \\ F_{T_v} \\ F_{T_g} \\ F_{T_2} \\ F_{T_3} \end{bmatrix}
$$

$$
\begin{pmatrix}
C^1_{T_s} & 0 & C^1_{(T_v)_1} & C^1_{(T_v)_2} & C^1_{(T_v)_3} & C^1_{T_g} & 0 & 0 & 0 & 0 & 0 \\
0 & C^2_{q_s} & C^2_{(T_v)_1} & C^2_{(T_v)_2} & C^2_{(T_v)_3} & C^2_{T_g} & 0 & 0 & 0 & 0 & 0 \\
C^3_{T_s} & C^3_{q_s} & C^3_{(T_v)_1} & 0 & 0 & C^3_{T_g} & 0 & 0 & 0 & 0 & 0 \\
C^4_{T_s} & C^4_{q_s} & 0 & C^4_{(T_v)_2} & 0 & C^4_{T_g} & 0 & 0 & 0 & 0 & 0 \\
C^5_{T_s} & C^5_{q_s} & 0 & 0 & C^5_{(T_v)_3} & C^5_{T_g} & 0 & 0 & 0 & 0 & 0 \\
C^6_{T_s} & C^6_{q_s} & C^6_{(T_v)_1} & C^6_{(T_v)_2} & C^6_{(T_v)_3} & C^6_{T_g} & C^6_{T_{-1}} & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & C^7_{T_g} & C^7_{T_{-1}} & C^7_{T_0} & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & C^8_{T_{-1}} & C^8_{T_0} & C^8_{T_1} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & C^9_{T_0} & C^9_{T_1} & C^9_{T_2} & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C^{10}_{T_1} & C^{10}_{T_2} & C^{10}_{T_3} \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & C^{11}_{T_2} & C^{11}_{T_3}
\end{pmatrix}
\times
\begin{bmatrix} \Delta T_s \\ \Delta q_s \\ \Delta (T_v)_1 \\ \Delta (T_v)_2 \\ \Delta (T_v)_3 \\ \Delta T_g \\ \Delta T_{-1} \\ \Delta T_0 \\ \Delta T_1 \\ \Delta T_2 \\ \Delta T_3 \end{bmatrix}
=
\begin{bmatrix} F_{T_s} \\ F_{q_s} \\ F_{(T_v)_1} \\ F_{(T_v)_2} \\ F_{(T_v)_3} \\ F_{T_g} \\ F_{T_{-1}} \\ F_{T_0} \\ F_{T_1} \\ F_{T_2} \\ F_{T_3} \end{bmatrix}
$$

canopy air space | pfts 1, 2, and 3 | snow layers -2, -1, and 0 | soil layers 1, 2, and 3

The matrix coefficients are indexed at top right by the row number (or equation) that they belong to and at bottom right by the column (or prognostic variable) that they correspond to.

Recall that CLM uses 10 soil layers, up to four pfts, and up to 5 snow layers in each grid cell by default. CLM adjusts the size of matrix *A* in every grid cell according to the actual number of pfts and snow layers. The matrix size can range from 11x11 for a column with no snow and no pfts (e.g., wetland, glacier, bare soil; *npft* equals 1 but $L + S$ equals 0 in such columns) up to 20x20 for a column with four pfts and 5 snow layers.

4. Steps Toward Implementation

A fortran routine based on SiB3 subroutine sibslv.F90 was written to fill the coefficients of the matrix of section 3 with realistic data from one time step of a single-point CLM simulation. The main routine calls a matrix solver (subroutine dgesv) and writes the solution as though one CLM time step has passed.

The fortran routine was originally tested in one column with one pft and no snow:

1. The heat capacities of vegetation and canopy air space were set to zero to mimic CLM assumptions. The matrix solution appeared reasonable but values were different from CLM output at the same time step.
2. Finite heat capacities were used for vegetation and canopy air space and the results changed mainly above ground as expected.
3. A $2\Delta t$ smoothing filter was used in Eq. 1c to Eq. 4c following the approach found in SiB3. The results changed mainly above ground because the smoothing was not used below ground.
4. The routine was changed to accommodate multiple pfts. T_s and q_s were made column level variables. The results did not change when setting *npft* = 1.

5. Solving for two or more identical pfts (*npft* > 1) gave same answers for each of the pfts as for the single pft in test #4.
6. Vegetation related variables were set to zero to test the matrix for the case of bare ground. The results changed mainly above ground as expected.
7. The routine was generalized to accommodate snow. The results did not change when *snl* was set to zero.
8. As this document was written, a few errors were found in the definitions of some matrix coefficients, so answers changed. However, the new results look just as reasonable as the old.
9. This new matrix solution will be linked to the CLM as a replacement to the original iterative solution. In CLM the matrix dimensions will be determined dynamically for variable numbers of pfts and snow layers to ensure maximum computational efficiency. Extensive tests will be performed with the new and the old codes to demonstrate that the new solution works correctly. Some of the tests described earlier in this section will be repeated. Also conservation tests for mass and energy will be performed.

5. Necessary Code Changes

List subroutines that were removed, added, or changed. List corresponding sections from Oleson *et al.* (2004) that become obsolete.

Keith mentioned that after phase chg in soils we adjust temps and/or fluxes? This consideration should be added to the discussion of how to apply limits to the matrix solution. Apply the limits recommended by Vidale & Stöckli (2005) (see Eq. B1)? Keep clm's current method of applying limits? Eg, now clm applies E_c limits within the iterative scheme, but we calc other fluxes after it and then solve soil moisture and update fluxes. Would it be cleaner to calc soil moisture first, then solve matrix with B1 limits to get the fluxes once?

6. To Do…

Add or just refer to Keith's figures such as 4.1, 5.1, 5.2, 6.1?

Ian (?) suggested that we compile with ATLAS (?)

Bibliography

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Add a SiB reference OR Ian's write-up?