Appendix A: Matrix expressions and numerical cost of the coupled-surface scheme

A1 Matrix expressions

Combing Eqs. (5), (6), and (10), the Newton scheme of the coupled-surface model proposed in this article can be written under block matrix form

$$\left(\begin{array}{c|c} A_{\mathrm{diag}} & A_{\mathrm{up}} \\ \hline A_{\mathrm{low}} & A_{\mathrm{s}} \end{array}\right)\left(\begin{array}{c} T_{\mathrm{int}} \\ \hline U_{\mathrm{s}} \end{array}\right) = \left(\begin{array}{c} B_{\mathrm{int}} \\ \hline B_{\mathrm{s}} \end{array}\right) \tag{A1}$$

with non-zero terms being

$$A_{\mathrm{diag}}(k,k) = \Delta z_{\mathrm{k}} c_{\mathrm{p_k}} + \Delta t \left(\frac{\lambda^{\mathrm{harm}}_{\mathrm{k}+\frac{1}{2}}}{\frac{\Delta z_{\mathrm{k}}}{2} + \frac{\Delta z_{\mathrm{k}+1}}{2}} + \frac{\lambda^{\mathrm{harm}}_{\mathrm{k}-\frac{1}{2}}}{\frac{\Delta z_{\mathrm{k}}}{2} + \frac{\Delta z_{\mathrm{k}-1}}{2}} \right) \tag{A2}$$

$$A_{\mathrm{diag}}(k,k-1) = -\Delta t \frac{\lambda^{\mathrm{harm}}_{\mathrm{k}-\frac{1}{2}}}{\frac{\Delta z_{\mathrm{k}}}{2} + \frac{\Delta z_{\mathrm{k}-1}}{2}} \tag{A3}$$

$$A_{\mathrm{diag}}(k,k+1) = -\Delta t \frac{\lambda^{\mathrm{harm}}_{\mathrm{k}+\frac{1}{2}}}{\frac{\Delta z_{\mathrm{k}}}{2} + \frac{\Delta z_{\mathrm{k}+1}}{2}} \tag{A4}$$

$$A_{\mathrm{up}}(N-1,1) = A_{\mathrm{low}}(1,N-1) = -\Delta t \frac{\lambda^{\mathrm{harm}}_{\mathrm{N}-\frac{1}{2}}}{\frac{\Delta z_{\mathrm{N}-1}}{2} + \frac{\Delta z_{\mathrm{N}}}{2}} \tag{A5}$$

$$A_{\mathrm{s}}(1,1) = \Delta z_{\mathrm{N}} c_{\mathrm{p_N}} + \Delta t \left(\frac{\lambda^{\mathrm{harm}}_{\mathrm{N}-\frac{1}{2}}}{\frac{\Delta z_{\mathrm{N}}}{2} + \frac{\Delta z_{\mathrm{N}-1}}{2}} + \frac{\lambda_{\mathrm{N}}}{\frac{\Delta z_{\mathrm{N}}}{2}} \right) \tag{A6}$$

$$A_{\mathrm{s}}(2,2) = \Delta t \left(\frac{\lambda_{\mathrm{N}}}{\frac{\Delta z_{\mathrm{N}}}{2}} \mathrm{d}_\tau T_{\mathrm{surf}} + L_{\mathrm{fus}} \mathrm{d}_\tau \dot{m} - \mathrm{d}_\tau H - \mathrm{d}_\tau L - \mathrm{d}_\tau L W_{\mathrm{out}} - -\mathrm{d}_\tau R \right) \tag{A7}$$

$$A_{\mathrm{s}}(1,2) = -\Delta t \frac{\lambda_{\mathrm{N}}}{\frac{\Delta z_{\mathrm{N}}}{2}} \mathrm{d}_\tau T_{\mathrm{surf}} \tag{A8}$$

$$A_{\mathrm{s}}(2,1) = -\Delta t \frac{\lambda_{\mathrm{N}}}{\frac{\Delta z_{\mathrm{N}}}{2}} \tag{A9}$$

$$B_{\mathrm{int}}(k) = \Delta z_{\mathrm{k}} c_{\mathrm{p_k}} T_{\mathrm{k}}^{n-1} + \Delta t \mathrm{SW}_{\mathrm{int,k}} \tag{A10}$$

$$B_{\mathrm{s}}(1) = \Delta z_{\mathrm{N}} c_{\mathrm{p_N}} T_{\mathrm{N}}^{n-1} + \Delta t \left(\mathrm{SW}_{\mathrm{int,N}} - \frac{\lambda_{\mathrm{N}}}{\frac{\Delta z_{\mathrm{N}}}{2}} \left(\mathrm{d}_\tau T_{\mathrm{surf}} \tau^{\mathrm{i}} - T_{\mathrm{s}}(\tau^{\mathrm{i}}) \right) \right) \tag{A11}$$

$$\begin{aligned} B_{\mathrm{s}}(2) = \Delta t \Big(& SW_{\mathrm{net}}^{\mathrm{surf}} + LW_{\mathrm{in}} - \frac{\lambda_{\mathrm{N}}}{\frac{\Delta z_{\mathrm{N}}}{2}} \left(T_{\mathrm{s}}(\tau^{\mathrm{i}}) - \mathrm{d}_\tau T_{\mathrm{surf}} \tau^{\mathrm{i}} \right) - L_{\mathrm{fus}} \left(m(\tau^{\mathrm{i}}) - \mathrm{d}_\tau m \tau^{\mathrm{i}} \right) \\ & + \left(H(\tau^{\mathrm{i}}) - \mathrm{d}_\tau H \tau^{\mathrm{i}} \right) + \left(L(\tau^{\mathrm{i}}) - \mathrm{d}_\tau L \tau^{\mathrm{i}} \right) + \left(R(\tau^{\mathrm{i}}) - \mathrm{d}_\tau R \tau^{\mathrm{i}} \right) + \left(LW_{\mathrm{out}}(\tau^{\mathrm{i}}) - \mathrm{d}_\tau LW_{\mathrm{out}} \tau^{\mathrm{i}} \right) \Big) \end{aligned} \tag{A12}$$

In the above expressions, T_{k}^{n-1} is the temperature of cell k at the previous time step, $\mathrm{SW}_{\mathrm{int,k}}$ is the quantity of shortwave radiation absorbed in cell k, and τ^{i} is the value of the fictitious variable τ at the start of the current non-linear iteration. The terms $T_{\mathrm{s}}(\tau^{\mathrm{i}})$, $H(\tau^{\mathrm{i}})$, etc, and $\mathrm{d}_\tau T_{\mathrm{surf}}$, $\mathrm{d}_\tau H$, etc, are the values of the surface temperature, sensible heat flux, etc, and their derivatives at the current τ^{i} estimation.

Among the different partial derivatives, $\mathrm{d}_\tau H$ and $\mathrm{d}_\tau L$ can be difficult to analytically derive. For that, we first note that the chain rule yields $\mathrm{d}_\tau H = \mathrm{d}_{T_{\mathrm{s}}} H \mathrm{d}_\tau T_{\mathrm{s}}$, and $\mathrm{d}_\tau L = \mathrm{d}_{T_{\mathrm{s}}} L \mathrm{d}_\tau T_{\mathrm{s}}$. Then, for the expression of H given in Appendix D we have:

$$\mathrm{d}_{T_{\mathrm{s}}} H = \rho_{\mathrm{a}} c_{\mathrm{p,a}} u \left(\mathrm{d}_{T_{\mathrm{s}}} C_{\mathrm{H}} (T_{\mathrm{a}} - T_{\mathrm{s}}) - C_{\mathrm{H}} \right) \tag{A13}$$

Moreover, the chain rule yields $\mathrm{d}_{T_{\mathrm{s}}} C_{\mathrm{H}} = \mathrm{d}_{\mathrm{Ri_b}} C_{\mathrm{H}} \mathrm{d}_{T_{\mathrm{s}}} \mathrm{Ri_b}$. In our case:

$$\mathrm{d}_{\mathrm{Ri_b}} C_{\mathrm{H}} = \frac{\kappa^2}{\ln\left(\frac{z}{z_0}\right)\left(\frac{z}{z_{0t}}\right)} \begin{cases} 0 & \text{if } \mathrm{Ri_b} < 0 \\ 50\mathrm{Ri_b} - 10 & \text{if } 0 \leq \mathrm{Ri_b} < 0.2 \\ 0 & \text{if } 0.2 \leq \mathrm{Ri_b} \end{cases} \tag{A14}$$

and

$$\mathrm{d}_{T_{\mathrm{s}}} \mathrm{Ri_b} = -\frac{g z_{\mathrm{a}}}{T_{\mathrm{a}} u^2} \tag{A15}$$

Similarly, for L, we have:

$$\mathrm{d}_{T_{\mathrm{s}}} L = \rho_{\mathrm{a}} L_{\mathrm{s}} u \left(\mathrm{d}_{T_{\mathrm{s}}} C_{\mathrm{E}} (q_{\mathrm{a}} - q_{\mathrm{s}}) - C_{\mathrm{E}} \mathrm{d}_{T_{\mathrm{s}}} q_{\mathrm{s}} \right) \tag{A16}$$

The derivative $\mathrm{d}_{T_{\mathrm{s}}} C_{\mathrm{E}}$ can be computed as the one of C_{H} through the chain rule and its dependence to $\mathrm{Ri_b}$. The derivative of q_{s} with respect to T_{s} can be easily obtained using the derivative of the saturated water vapor pressure, which is given by the Clausius-Clapeyron relation.

Appendix C: Finite Element Method scheme

In this paper, we focus on the FVM for spatial discretization. However, the heat budget equation could also be spatially discretized with the FEM. Indeed, the FEM naturally includes a node at the surface, and thus possesses a surface temperature, which helps to tightly couple the SEB to the interior of the snowpack/glacier. This strategy is for instance employed in the SNOWPACK model (Bartelt and Lehning, 2002; Wever et al., 2020). Specifically, in SNOWPACK, the coupled SEB is introduced as a top Robin boundary condition.

The goal of this appendix is to briefly present how the techniques presented in the main part of the manuscript (namely the use of fictitious variable and of a Schur-complement) can be used to implement a tightly-coupled FEM model.

C1 Expression of the heat equation in FEM

We consider the mesh of the domain to be discretized into N 1D elements (the direct equivalent of the cells in FVM) and thus of $N+1$ nodes (the end-points of the elements). As classically done with FEM (Pepper and Heinrich, 2005), we assume the temperature field to be a linear combination of basis functions φ_j, i.e. $T(z,t) = \sum_{k=1}^{N} T_j(t)\varphi_j(z)$. Here, we use basic linear elements. In this framework, $T_j(t)$ corresponds to the nodal value of the temperature field (which evolves over time) and the basis functions $\varphi_j(z)$ are piece-wise linear functions, valued 1 at node j and 0 at all other nodes. The standard Galerkin form (Pepper and Heinrich, 2005) of the internal heat budget (Eq. (1)) is:

$$\forall i \quad \sum_j \mathrm{d}_t T_j \int_\Omega c_\mathrm{p}\varphi_j\varphi_i \mathrm{dL} + \sum_j T_j \int_\Omega \lambda \nabla\varphi_j \cdot \nabla\varphi_i \mathrm{dL} = \int_\Omega Q\varphi_i \mathrm{dL} + F_\mathrm{s}\varphi_i(\mathrm{s}) \tag{C1}$$

where Ω represents the domain of simulation, F_s is the energy fluxes entering at the top of the domain (i.e. G), and $\varphi_i(\mathrm{s})$ is the basis function φ_i evaluated at top of the domain. We note that similarly to the FVM case, the temperature at the top of the domain presents a regime change whether the surface is melting or not. To handle this, we rely on the fictitious variable τ, i.e. $T_\mathrm{s} = T_\mathrm{s}(\tau)$. The vector of unknowns, denoted U, is thus composed of the internal temperatures and of the surface fictitious variable. Finally, we have not included any bottom energy flux to lighten the notation, but it could be included easily. Once temporally discretized with a Backward Euler scheme and linearized, the problem can be expressed in matrix form $AU^n = B$, with $A = (M + \Delta t K + \Delta t L)J_T$ and $B = MT^{n-1} + \Delta t Q + \Delta t F$ (T^{n-1} being the vector of temperature from the previous time step), and

$$M(i,j) = \int_\Omega c_\mathrm{p}\varphi_j\varphi_i \mathrm{dL} \tag{C2}$$

$$K(i,j) = \int_\Omega \lambda \nabla\varphi_j \cdot \nabla\varphi_i \mathrm{dL} \tag{C3}$$

$$L(N+1,N+1) = -d_\tau SEB + L_{\text{fus}} d_\tau \dot{m} \tag{C4}$$

$$J_T(i,i) = \begin{cases} 1 & \text{if } i \leq N \\ d_\tau T_{\text{s}} & \text{else} \end{cases} \tag{C5}$$

$$Q(i) = \int_\Omega Q \varphi_i \mathrm{dL} \tag{C6}$$

and

$$F(N+1) = SEB(\tau^i) - d_\tau SEB \tau^i - \dot{m} + L_{\text{fus}} \left(d_\tau \dot{m} \tau^i \right) \tag{C7}$$

where SEB and $d_\tau SEB$ corresponds to the atmospheric fluxes in the SEB and their derivatives with respect to τ at the current iteration, and $\dot{m}$ and $d_\tau \dot{m}$ are the melting rate and its derivative at the current iteration. In the equations above, only the non-zero terms have been given.

As in the FVM case, this system is composed of a linear-part (the interior, corresponding to the first $N-1$ equations) and a non-linear part (the surface, corresponding to the last two equations). Its solving can thus be accelerated using a Schur-complement technique (Section 4.1.1) by breaking the matrix A into four blocks: a constant $(N-1) \times (N-1)$ diagonal A_{diag} block, a constant $(N-1) \times 2$ vertical A_{up} block, a constant $2 \times (N-1)$ horizontal A_{low} block, and a 2×2 diagonal block A_{s} to be re-computed at each non-linear iteration.

C2 The rest of the model

After solving the coupled heat budgets with FEM, we obtain a nodal temperature field. Since conserved quantities, such as energy or mass, are defined element-wise in snowpack/glacier FEM models (Bartelt and Lehning, 2002), the nodal temperature field needs to be converted into an element-wise energy field. We note that this also defines an element-wise temperature field, where the temperature of an element is simply the average of the nodal temperatures at its end. This element-wise energy field can then be used to simulate melt/refreeze, liquid water percolation, and to remesh the domain using the same routines as in FVM models.

Once all routines for a given time step have been performed, we are left with an element-wise temperature field that needs to be converted back to a nodal temperature field, as required for the FEM. However, this conversion is not straightforward.

First, as we have N element-wise temperatures to transform into $N+1$ nodal temperatures, the problem is not properly closed and an extra (arbitrary) constraint needs to be added. This could, for instance, be setting the surface temperature to the value computed in the SEB. Furthermore, even after choosing an extra constraint to close the problem, the element-wise to node-wise transformation can produce spurious oscillations in the nodal field even if the element-wise field is monotonous (in other words, the transformation does not respect a form of discrete maximum principle; Ciarlet and Raviart, 1973). It is therefore not possible to derive an optimal scheme for this transformation that would (i) not modify the element-wise temperature field and (ii) not create spurious oscillations in the node-wise temperature field.

As spurious oscillations in the temperature field would affect the estimation of the temperature gradients that are used in snowpack models to estimate metamorphism (e.g. Bartelt and Lehning, 2002; Vionnet et al., 2012), it seems preferable to rather allow the modification of the element-wise temperature field. That being said, such a strategy implies a spatial re-distribution of energy between elements that is not motivated by any underlying physical mechanism. We note that the SNOWPACK model handles this element to node transformation during a phase change step after the liquid percolation scheme, and does so without creating large spurious temperature oscillations.

Unfortunately, it is not possible to directly implement the SNOWPACK scheme in our toy-model, as the sequential treatment is not the same. Moreover, we did not manage to derive a scheme that performs this element to node transformation without affecting the surface temperature. Thus, in our numerical simulations, the FVM and FEM models yield different results. In the absence of an analytical solution, a direct comparison of the FEM and FVM implementations remains impossible.

Appendix E: Stability Analysis

Here, we present the derivation of the criteria for the numerical stability of the different numerical schemes presented in the paper. We follow the proof classically used to show the (un)conditional stability of the Forward and Backward Euler method (Butcher, 2008). Notably, the proof relies on a linearized version of the system of equations. As the system needs to be linearized, we cannot account for the potential melting of the surface. Under this consideration, the atmospheric fluxes in the SEB (long-wave radiations, turbulent fluxes, etc) are simply expressed as a linear function of the surface temperature T_s, i.e. as $fT_\mathrm{s} + b$, where f and b are constant scalars expressed in $\mathrm{J\,s^{-1}\,m^{-2}\,K^{-1}}$ and in $\mathrm{J\,s^{-1}\,m^{-2}}$, respectively.

Also, for simplicity, we consider a system composed of only one cell and its surface. The problem could be generalized to more cells, but it would make the computation more cumbersome and is not crucial as we are considering numerical instabilities that develop in the vicinity of the surface.

E1 Standard skin-layer formulation (Class 2)

To compute the surface temperature T_s^{n+1} at time step $n+1$, we use the discretized Surface Energy Balance (SEB):

$$fT_\mathrm{s}^{n+1} + b + \frac{2\lambda}{\Delta z}\left(T_\mathrm{s}^{n+1} - T_\mathrm{i}^{n}\right) = 0 \tag{E1}$$

where the first two terms corresponds to the sum of outgoing/incoming atmospheric fluxes, and the last term to the subsurface heat conduction flux. Here, λ is the thermal conductivity of the internal cell and Δz its thickness. Note that the internal temperature T_i^{n} is taken from the previous time step. To compute the internal temperature at time step $n+1$, we use the heat budget of the internal cell:

$$\Delta z c_p T_\mathrm{i}^{n+1} + \Delta t \frac{2\lambda}{\Delta z}\left(T_\mathrm{i}^{n} - T_\mathrm{s}^{n+1}\right) = \Delta z c_p T_\mathrm{i}^{n} \tag{E2}$$

where the second term of the LHS is the opposite of the subsurface conduction flux appearing in the SEB (for energy conservation), and c_p is the heat capacity of the internal cell. The two above equations can be expressed in matrix form $MU_{n+1} = NU_n + B$, with U_n the solution vector $[T_\mathrm{s}, T_\mathrm{i}]^T$ at the n^{th} time step and

$$M = \begin{bmatrix} 1 & 0 \\ -\frac{2\Delta t\lambda}{c_p \Delta z^2} & 1 \end{bmatrix} \tag{E3}$$

$$N = \begin{bmatrix} 0 & \frac{2\lambda}{2\lambda + \Delta z f} \\ 0 & 1 - \frac{2\Delta t\lambda}{c_p \Delta z^2} \end{bmatrix} \tag{E4}$$

and $B = [-\frac{\Delta z b}{\Delta z f + 2\lambda}, 0]^T$. We thus have, $U_{n+1} = QU_n + M^{-1}B$, with

$$Q = M^{-1}N = \begin{bmatrix} 0 & \frac{2\lambda}{2\lambda+\Delta z f} \\ 0 & 1 - \Delta t \frac{2\lambda}{c_p \Delta z^2} \frac{\Delta z f}{2\lambda+\Delta z f} \end{bmatrix} \tag{E5}$$

By recursion, it follows that $U_n = Q^n U_0 + M^{-n} B$. The numerical scheme is deemed stable if $\lim_{n\to\infty} Q^n = 0$. This is achieved if:

$$|1 - \Delta t \frac{2\lambda}{c_p \Delta z^2} \frac{\Delta z f}{2\lambda + \Delta z f}| < 1 \tag{E6}$$

which after some computation yields a criterion of the time step Δt:

$$\Delta t < \Delta t_{\mathrm{crit}} = \frac{c_p \Delta z}{\lambda} \frac{2\lambda + \Delta z f}{f} \tag{E7}$$

The (linearized) standard skin-layer is thus only conditionally stable. The stability criterion is relaxed with increasing heat capacity (c_p) and increasing cell size (Δz), and is made more restrictive with increasing thermal conductivity (λ) or if the SEB is more sensitive to changes in the surface temperature (f term).

E2 Coupled-surface formulation

Similarly, for a one cell system, the coupled-surface equations, after linearization, write:

$$f T_{\mathrm{s}}^{n+1} + b + \frac{2\lambda}{\Delta z} \left(T_{\mathrm{s}}^{n+1} - T_{\mathrm{i}}^{n+1} \right) = 0 \tag{E8}$$

for the SEB, and

$$\Delta z c_p T_{\mathrm{i}}^{n+1} + \Delta t \frac{2\lambda}{\Delta z} \left(T_{\mathrm{i}}^{n+1} - T_{\mathrm{s}}^{n+1} \right) = \Delta z c_p T_{\mathrm{i}}^{n} \tag{E9}$$

for the cell's heat budget. These two equations can be cast into the matrix form $MU_{n+1} = NU_n + B$, with $B = [-\frac{\Delta z b}{\Delta z f + 2\lambda}, 0]^T$,

$$M = \begin{bmatrix} 1 & \frac{-2\lambda}{2\lambda+\Delta z f} \\ -\frac{2\Delta t \lambda}{c_p \Delta z^2 + 2\lambda \Delta t} & 1 \end{bmatrix} \tag{E10}$$

and

$$N = \begin{bmatrix} 0 & 0 \\ 0 & \frac{c_p \Delta z^2}{c_p \Delta z^2 + 2\lambda \Delta t} \end{bmatrix} \tag{E11}$$

We thus have $U_n = Q^n U_0 + M^{-n} B$, with:

$$Q = \begin{bmatrix} 0 & \frac{2\lambda}{2\lambda+\Delta z f} \frac{c_p \Delta z^2}{c_p \Delta z^2 + 2\lambda \Delta t} \\ 0 & \frac{c_p \Delta z^2}{c_p \Delta z^2 + 2\lambda \Delta t} \end{bmatrix} \tag{E12}$$

The numerical scheme is deemed stable if $\lim_{n\to\infty} Q^n = 0$. This is always achieved, as $\frac{c_p \Delta z^2}{c_p \Delta z^2 + 2\lambda \Delta t} < 1$. Thus, the surface-coupled scheme is unconditionally stable.

E3 Non-conservative skin-layer formulation

For the non-conservative skin-layer formulation (see Section 6.4), we start with the linearized discrete SEB:

$$f T_{\mathrm{s}}^{n+1} + b + \frac{2\lambda}{\Delta z} \left(T_{\mathrm{s}}^{n+1} - T_{\mathrm{i}}^{n} \right) = 0 \tag{E13}$$

Using the surface temperature T_{s}^{n+1} as a Dirichlet condition for the internal energy budget, we thus have

$$\Delta z c_p T_{\mathrm{i}}^{n+1} + \Delta t \frac{2\lambda}{\Delta z} \left(T_{\mathrm{i}}^{n+1} - T_{\mathrm{s}}^{n+1} \right) = \Delta z c_p T_{\mathrm{i}}^{n} \tag{E14}$$

These two equations can be cast into the matrix form $M U_{n+1} = N U_n + B$, with $B = [-\frac{\Delta z b}{\Delta z f + 2\lambda}, 0]^T$,

$$M = \begin{bmatrix} 1 & 0 \\ -\frac{2\Delta t \lambda}{c_p \Delta z^2 + 2\lambda \Delta t} & 1 \end{bmatrix} \tag{E15}$$

and

$$N = \begin{bmatrix} 0 & \frac{2\lambda}{2\lambda+\Delta z f} \\ 0 & \frac{c_p \Delta z^2}{c_p \Delta z^2 + 2\lambda \Delta t} \end{bmatrix} \tag{E16}$$

We thus have $U_n = Q^n U_0 + M^{-n} B$, with:

$$Q = \begin{bmatrix} 0 & \frac{2\lambda}{2\lambda+\Delta z f} \\ 0 & X \end{bmatrix} \tag{E17}$$

where $X = \frac{2\lambda \Delta t \frac{2\lambda}{2\lambda+\Delta z f} + c_p \Delta z^2}{2\Delta t \lambda + c_p \Delta z^2}$. The scheme is deemed stable if $|X| < 1$.

As $\frac{2\lambda}{2\lambda+\Delta z f} < 1$, we always have that $2\lambda \Delta t \frac{2\lambda}{2\lambda+\Delta z f} + c_p \Delta z^2 < 2\Delta t \lambda + c_p \Delta z^2$, and thus that the scheme is unconditionally stable. That being said, we recall that this scheme is not energy conservative and can lead to large errors.

E4 No-surface formulation (Class 1)

Finally, we note that the linearized No-surface formulation corresponds to a classic heat equation with a Backward Euler time integration. As demonstrated elsewhere in the literature (e.g. Butcher, 2008), it is unconditionally stable.