Coupled FEM for ground heat recovery with ice formation

Energy-conservative thermo-hydraulic flow with conforming 1D–3D pipe coupling

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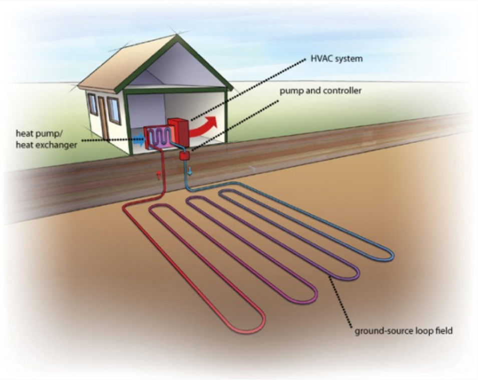
Why this problem

- Ground heat exchangers now run cold enough to freeze the soil by design
- Pore ice: zero-curtain latent heat, cryo-suction, permeability collapse
- Standard tools: soil = pure conductor, miss it
- Worth getting right: ground/seasonal source cuts heating electricity 25–50% vs. conventional, up to 44% vs. air-source (EPA/DOE)



Gap: open FEM coupling ice-aware flow with embedded pipes

Coupled system with phase change

Fields: h (head), T_s (soil temp.), T_p (pipe temp.)

Richards (flow in porous media): water in soil Ω

$$\partial_t \theta_\ell + \nabla \cdot \boldsymbol{q} = 0, \quad \boldsymbol{q} = -K(\nabla h + \mathbf{e}_z)$$

Heat: soil Ω (enthalpy form)

$$\partial_t H - \nabla \cdot (k_{\text{eff}} \nabla T_s) + \nabla \cdot (\boldsymbol{q}\, T_s) = -(T_s|_\Gamma - T_p)\, h_Z\, \delta_\Gamma$$

Heat: pipe Γ (1D advection–diffusion)

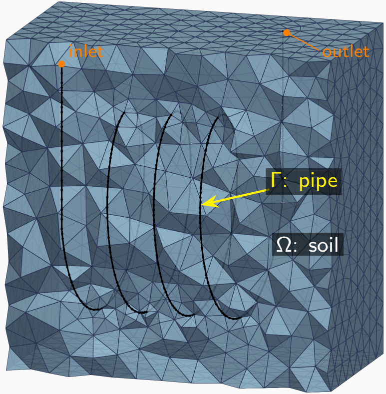
$$\partial_t T_p + \partial_s T_p - \partial_{ss} T_p = +(T_s|_\Gamma - T_p)\, h_Z$$

- $K(h, T_s)$: hydraulic conductivity
- $k_{\text{eff}}(h, T_s)$: effective thermal conductivity
- $H(h, T_s)$: volumetric enthalpy (carries latent heat)

$(T_s - T_p)\, h_Z$ couples soil $(-)$ and pipe $(+)$ with opposite signs (δ_Γ: line source on Γ) $\Rightarrow$ energy conserved

Domains and complete variational form

Γ_{top}: Dirichlet



Γ_{bot}: geothermal flux

Find (h, T_s, T_p), Dirichlet h, T_s on Γ_{top}, T_p at inlet;
$\forall\,(w_h, w_s, w_p)$:

$$\langle \partial_t \theta_\ell, w_h \rangle_\Omega + \langle K\, \nabla h, \nabla w_h \rangle_\Omega = 0$$

$$\langle \partial_t H, w_s \rangle_\Omega + \langle k_{\text{eff}} \nabla T_s, \nabla w_s \rangle_\Omega + \langle K\, \nabla h\, T_s, \nabla w_s \rangle_\Omega + \langle T_s - T_p, w_s \rangle_\Gamma = \langle q_g, w_s \rangle_{\Gamma_{\text{bot}}}$$

$$\langle \partial_t T_p, w_p \rangle_\Gamma + \langle \partial_s T_p, w_p \rangle_\Gamma + \langle \partial_s T_p, \partial_s w_p \rangle_\Gamma - \langle T_s - T_p, w_p \rangle_\Gamma = 0$$

Material laws: top to bottom

Start from the three coefficients (plotted next); each unfolds until everything is evaluable from (h, T_s).

Hydraulic K

$$K = K_{\mathrm{sat}}\, k_r$$

$$k_r = S_{\mathrm{eff}}^{\ell}\left[1-(1-S_{\mathrm{eff}}^{1/m})^m\right]^2$$

$$S_{\mathrm{eff}} = \frac{\theta_\ell-\theta_r}{\phi_{\mathrm{eff}}-\theta_r}$$

$$K_{\mathrm{sat}} = \frac{\rho_w g}{\mu(T_s)}\, k_{\mathrm{int}}^{\mathrm{eff}}$$

$$k_{\mathrm{int}}^{\mathrm{eff}} = k_{\mathrm{int}}^{\mathrm{thaw}}\, \frac{\phi_{\mathrm{eff}}^3/(1-\phi_{\mathrm{eff}})^2}{\phi^3/(1-\phi)^2}$$

Thermal k_{eff}

$$k_{\mathrm{eff}} = k_s^{1-\phi}\, k_l^{\theta_\ell}\, k_i^{\theta_i}\, k_a^{\theta_a}$$

geometric (Lichtenecker) mean

Enthalpy H

$$H = (\rho c)_{\mathrm{eff}}\, T_s + \rho_w L_f\, \theta_\ell$$

$$(\rho c)_{\mathrm{eff}} = (1-\phi)\rho c_s + \theta_\ell \rho c_l + \theta_i \rho c_i$$

sensible + latent (freeze stiffness)

⇓ all reduce to the phase fractions

$$\theta_\ell = \theta_r + (\phi-\theta_r)\, S_e(\psi_{\mathrm{tot}}),\quad \theta_i = \max(\theta_w^{\mathrm{cap}} - \theta_\ell, 0),\quad \theta_a = \max(\phi - \theta_w^{\mathrm{cap}}, 0),\quad \phi_{\mathrm{eff}} = \phi - \theta_i$$

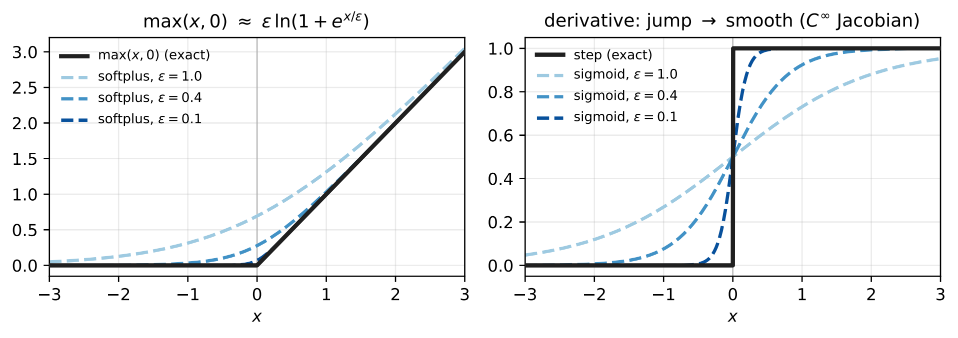
⇓ evaluable from (h, T_s): additive suction + van Genuchten retention

$$\psi_{\mathrm{cap}} = \max(-h, 0),\quad \psi_{\mathrm{frz}} = \max(H_c(T_m - T_s), 0),\quad \psi_{\mathrm{tot}} = \psi_{\mathrm{cap}} + \psi_{\mathrm{frz}}$$

$$S_e(\psi) = \left[1+(\alpha\psi)^n\right]^{-m},\quad m = 1-\frac{1}{n},\qquad \theta_w^{\mathrm{cap}} = \theta_r + (\phi-\theta_r)\, S_e(\psi_{\mathrm{cap}})$$

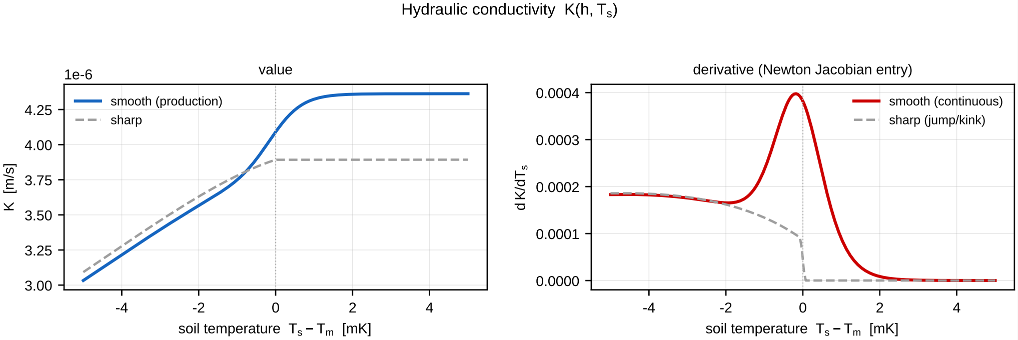
max **is not smooth**

Smoothing the kink: max vs softplus



- Softplus replaces the kink: $\max(x, 0) \approx \varepsilon \ln\left(1 + e^{x/\varepsilon}\right)$
- Its derivative is the sigmoid $\left(1 + e^{-x/\varepsilon}\right)^{-1}$: no jump $\Rightarrow$ C^{∞} Jacobian, robust Newton
- $\varepsilon \to 0$ recovers the exact max: smaller ε = sharper kink, stiffer Jacobian

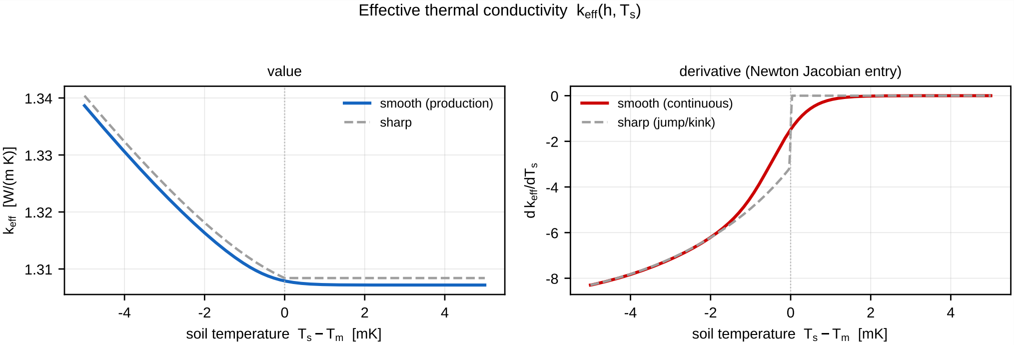
Nonlinearity 1: hydraulic conductivity $K(h, T_s)$



- van Genuchten $S_e(h)$, Mualem k_r: fractional powers
- freezing suction $\max(\cdot, 0)$ (softplus when smoothed); branch $\theta_\ell = \min(\text{capillary}, \text{freezing})$
- Kozeny–Carman collapse $\phi_{\text{eff}} = \phi - \theta_i$: ice chokes flow

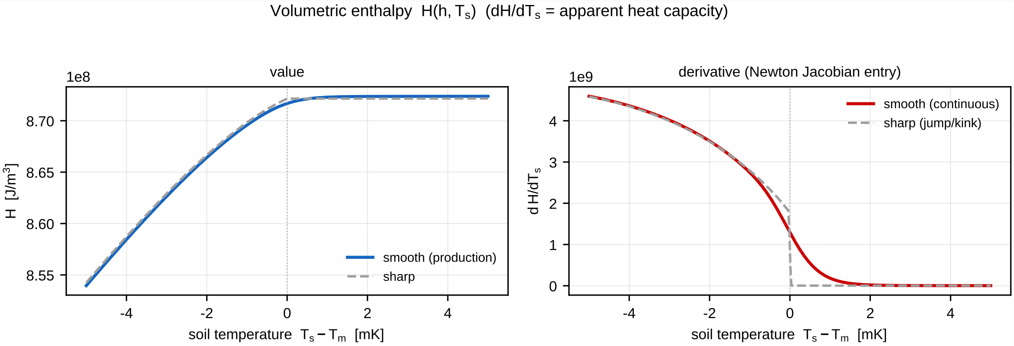
$\psi_{\text{tot}} = \max(-h, 0) + \max(H_c(T_m - T_s), 0)$ couples h and T_s into every coefficient

Nonlinearity 2: thermal conductivity $k_{\text{eff}}(h, T_s)$



- phase fractions $\theta_\ell, \theta_i, \theta_a$: carry the max / min kinks
- Lichtenecker geometric mix $k_s^{1-\phi}\, k_\ell^{\theta_\ell}\, k_i^{\theta_i}\, k_a^{\theta_a}$
- jumps across T_m as liquid (k_ℓ) turns to ice (k_i)

Nonlinearity 3: volumetric enthalpy $H(h, T_s)$



- latent term $\rho_w L_f \theta_\ell(h, T_s)$: steep dH/dT_s at T_m (the stiffness)
- $(\rho c)_{\text{eff}}$ weighting; same freezing curve θ_ℓ (max / min, softplus)
- zero-curtain plateau $\Rightarrow$ enthalpy form + adaptive Δt

Variational setting and BCs

Primal H^1, order 2, monolithic (h, T_s, T_p). Dirichlet in the space; zero-flux natural.

```
V_h  = H1(mesh, order=2, dirichlet="top")
V_Ts = H1(mesh, order=2, dirichlet="top")
fes  = V_h * V_Ts * V_Tp                       # V_Tp: glued pipe, next slide
(h, Ts, Tp), (wh, wTs, wTp) = fes.TnT()
```

Soil residual, single `BilinearForm`, Backward Euler (pipe + coupling added next):

```
R += C_cf*(h - h_n)/dt * wh * dx                     # Richards storage
R += InnerProduct(K_cf*grad(h), grad(wh)) * dx       # Darcy
R += K_cf*InnerProduct(ez, grad(wh)) * dx            # gravity
R += (H_new - H_old)/dt * wTs * dx                   # enthalpy storage
R += k_eff*InnerProduct(grad(Ts), grad(wTs)) * dx    # conduction
R += -rho_w*c_w*InnerProduct(q_D*Ts, grad(wTs))*dx   # advection
R += -q_geo * wTs * ds("bottom")                     # geothermal Neumann
```

1D–3D coupling: NGSolve code

Glue the 1D wire into the 3D box: shared nodes

```
shape   = Glue([box, pipe_wire])       # pipe nodes -> tet vertices
gamma   = mesh.BBoundaries("gamma")    # the glued pipe edges
V_Tp    = H1(mesh, order=2, dirichlet_bbbnd="inlet", definedon=gamma)
dx_pipe = dx(gamma)                    # 1D measure on Gamma
```

Double trace 3D $\to$ 1D, four symmetric terms complete R:

```
Ts_on_gamma = Ts.Trace().Trace()
R +=  h_Z * Tp          * wTp                  * dx_pipe   # +q on pipe
R += -h_Z * Ts_on_gamma * wTp                  * dx_pipe   #    "
R += -h_Z * Tp          * wTs.Trace().Trace()  * dx_pipe   # -q on soil
R +=  h_Z * Ts_on_gamma * wTs.Trace().Trace()  * dx_pipe   #    "
```

Soil + pipe + coupling: the monolithic residual R is now complete.

Monolithic Newton and enthalpy time stepping

```
with TaskManager():
    Newton(R, gfu, freedofs=fes.FreeDofs(),
           maxerr=1e-6, maxit=20, dampfactor=0.9, inverse="pardiso")
```

Line-search (3D), `pardiso`, rollback, stationary solve first.

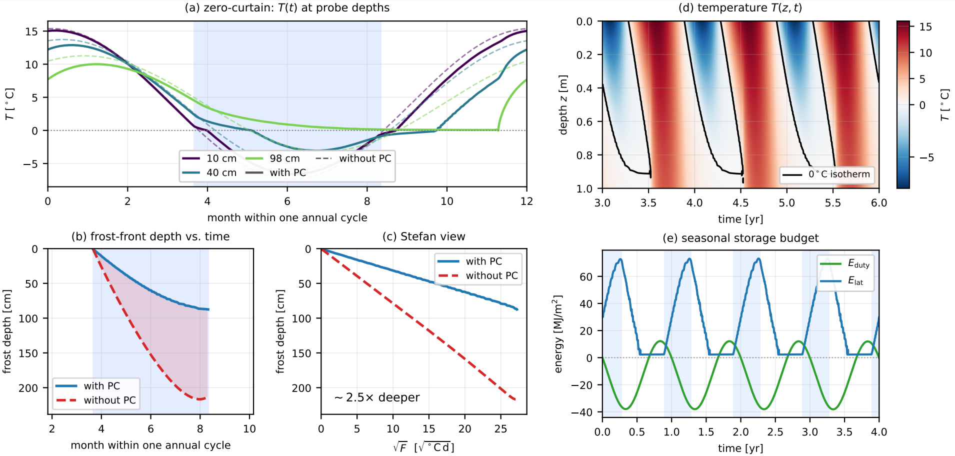
Time stepping: enthalpy storage $T \approx T_m$ but H jumps; $(H^{n+1} - H^n)/\Delta t$ keeps Backward Euler exact across the plateau.

```
H_new = cons.enthalpy(h, Ts, pcf).Compile()  # H_old at (h_n, T_n)
```

Adaptive Δt, tighten near the front:

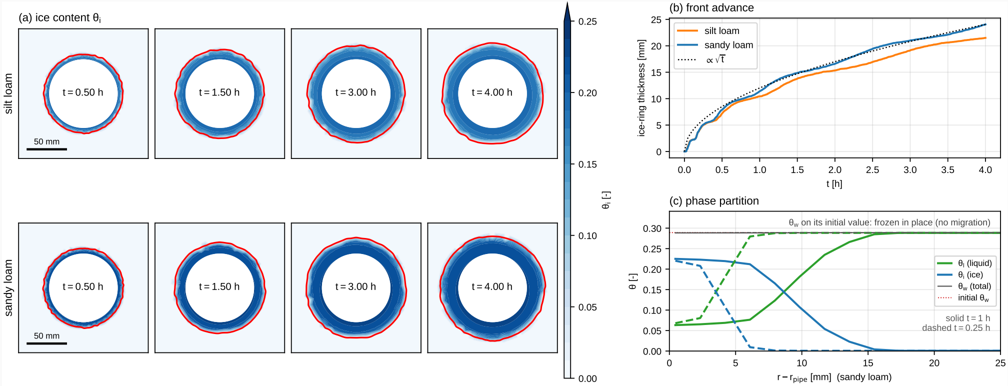
```
if   T_min_C > 0.5: dt_max = 300.0
elif T_min_C > 0.3: dt_max = 10.0
else:               dt_max = 1.5
```

Results: 1D seasonal column (decade)



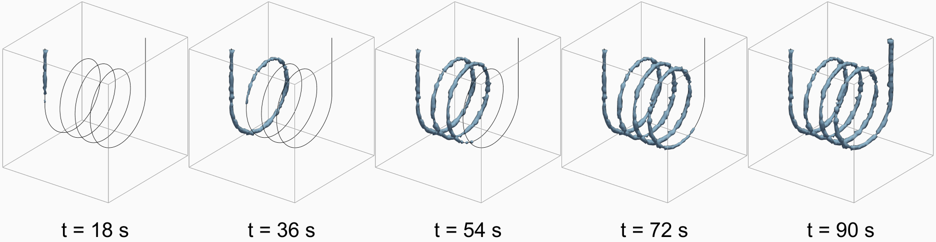
Latent heat halves frost depth (88 vs 216 cm); zero-curtain plateau; seasonal latent-ice buffer (74 MJ/m^2).

Results: 2D freezing front (two soils)



$\sqrt{t}$ Stefan front; ice ring ≈24 mm sandy / 21 mm silt; water conserved.

Results: 3D embedded helix

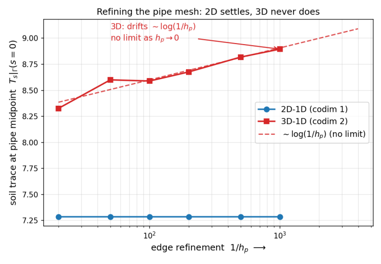


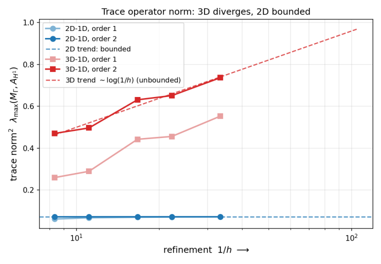
Ice crust nucleates at the cold inlet, sheaths Γ by ∼77 s. Energy $\varepsilon_E = 2.9 \times 10^{-3}$, mass $\varepsilon_M = 9.1 \times 10^{-6}$.

Open question: is the coupling mesh-convergent?

- Line in 3D = codim 2: $\log r$ singularity $\Rightarrow$ $T_s \in H^{1-\varepsilon}$, line trace is an unbounded functional
- *Top:* refine $h_p \Rightarrow$ pointwise trace drifts $\sim \log(1/h_p)$
- *Bottom:* trace norm$^2 = \lambda_{\max}(M_\Gamma, A_{H^1})$ diverges (mesh-only, no solve)
- `Trace().Trace()` = this non-convergent object
- 2D–1D (codim 1) bounded in both

Reported results stand: validated by conservation + $\sqrt{t}$ at fixed mesh.

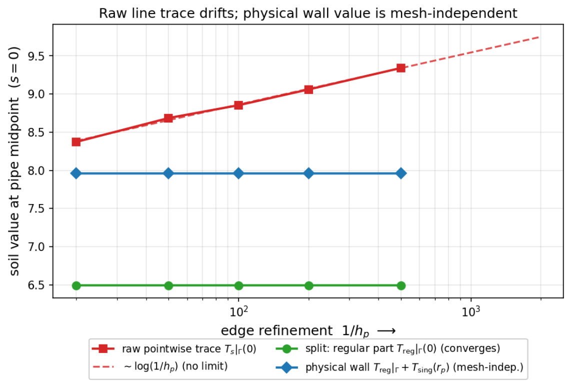




A fix: singularity splitting

- Line source = 2D point source in the ⊥ plane: $T_s = T_{\mathrm{sing}} + T_{\mathrm{reg}}$
- $T_{\mathrm{sing}}(r) = -\dfrac{Q(s)}{2\pi k_{\mathrm{eff}}} \log r$ carries the whole singularity (r: dist. to Γ)
- Remainder T_{reg} harmonic across Γ, in H^1: its line trace converges
- Couple via $T_{\mathrm{reg}}|_\Gamma + T_{\mathrm{sing}}(r_p)$: the physical wall value, mesh-independent

Verified by convergence, not the eigenvalue test: splitting changes *what* we trace, not the trace operator on V_h (its norm still diverges).



Cost and outlook

	1D decade	2D	3D helix
DOFs	322	24 448	64 334
Wall time	cheap	$\sim$4.5–6.1 h	$\sim$4.9 h

- 3D: 4.9 h wall for 432 s physics, $\sim$40$\times$ slower than real time; decades $\times$ scenarios $\Rightarrow$ full-order model impractical
- **Fix (accuracy):** convergent coupling via averaged-radius trace or singularity splitting (shown); SUPG / DG-upwind for pipe advection at $\mathrm{Pe}_h > 1$
- **Faster full-order:** HDG: static condensation (fewer global DOFs) + native upwinding; matrix-free assembly, parallel solve
- **Long-term prediction:** reduced-order / operator-learning surrogate (e.g. DeepONet) calibrated on these full-order references

Thank you!

References

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- M. Dall'Amico et al. (2011), *The Cryosphere*: energy-conserving model of freezing variably-saturated soil
- C. D'Angelo & A. Quarteroni (2008), *Math. Models Methods Appl. Sci.*: coupling of 1D and 3D diffusion–reaction equations
- I. G. Gjerde, K. Kumar & J. M. Nordbotten (2020), *Comput. Geosci.*: singularity removal for coupled 1D–3D flow