Benchmark test for the heat conduction equation with phase change: 3d-axisymmetric problem of soil freezing around a BHE

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December 20, 2022

1 Heat conduction equation with phase change

The initial-boundary value problem for the heat equation equation with phase (water-to-ice) change reads:

$$\left((\varrho c_p)^{\text{eff}} - \ell \varrho_{\text{IR}} \frac{\mathrm{d}\phi_{\text{I}}}{\mathrm{d}T}\right) \frac{\partial T}{\partial t} - \lambda^{\text{eff}} \Delta T - (\lambda_{\text{IR}} - \lambda_{\text{LR}}) \frac{\mathrm{d}\phi_{\text{I}}}{\mathrm{d}T} |\nabla T|^2 = Q_T(\mathbf{x}, t) \quad \text{in } \Omega, \tag{1}$$

where $T = T(\mathbf{x}, t)$ is the temperature distribution subject to the initial and boundary conditions

$$\begin{cases} T = T_0(\mathbf{x}) & \text{in } \Omega \quad \text{(IC)}, \\ T = T_1(t) & \text{on } \Gamma_D \quad \text{(BC)}. \end{cases} \tag{2}$$

Equation (1) is the extended version of a classical heat conduction equation and is capable of modeling ice formation and melting in saturated porous medium. In the OpenGeoSys documentation it is sometimes termed the "T+freezing" equation.

In (1), on has

$$(\varrho c_p)^{\text{eff}} = (1 - \phi)\varrho_{\text{SR}} c_{p\text{S}} + (\phi - \phi_{\text{I}})\varrho_{\text{LR}} c_{p\text{L}} + \phi_{\text{I}} \varrho_{\text{IR}} c_{p\text{I}},$$
$$\lambda^{\text{eff}} = (1 - \phi)\lambda_{\text{SR}} + (\phi - \phi_{\text{I}})\lambda_{\text{LR}} + \phi_{\text{I}} \lambda_{\text{IR}},$$

where ϕ is the porosity, function $\phi_{\text{I}} := \phi_{\text{I}}(T) = \phi S_{\text{I}}(T)$ models the ice volume fraction, where, in turn,

$$S_{\text{I}}(T) := \frac{1}{1 + e^{k(T - T_{\text{m}})}}, \quad k > 1,\ T_{\text{m}} = 273.15\,\text{K}, \tag{3}$$

is the so-called ice-fraction indicator function which aims at distinguishing between the liquid and the ice phases of the fluid (values 0 and 1, resp.) within the physical domain Ω, as well as at tracing these phases evolution in time. It is a regularized counterpart of the corresponding Heaviside-like function, see Figure 1. Also in (1), parameter ℓ is the so-called heat of fusion of ice, whereas all other parameters in (1) are standard ones related to the classical THM modeling of processes in saturated porous medium.

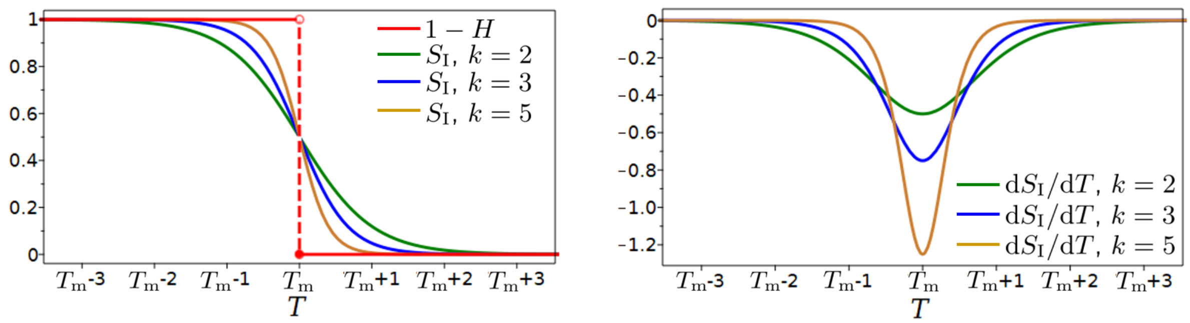


Figure 1: On the left: plots of the Heaviside-like ice-fraction indicator function (denoted as $1-H$) and its regularized counterpart S_{I}; on the right: plots of the first-order derivative of S_{I}.

2 3d-axisymmetric problem of soil freezing around a BHE

In this section, using (1)–(2), we model heat transfer process, focusing specifically on ice formation, in a cylindrical soil specimen around a borehole heat exchanger (BHE) – see the left plot in Figure 2 – which contains a refrigerant of sub-zero temperature. This (negative) temperature is used to prescribe a Dirichlet boundary condition on the specimen boundary adjacent to the BHE, what triggers cooling and consequent freezing of water-saturated soil whose initial temperature was assumed positive.

Simulations are performed using both our OpenGeoSys platform (in the following, simply termed OGS) and the FreeFem++ open source finite element code [1], thus enabling verification of the developed for solving (1)-(2) codes. Due to the domain and problem symmetry, we reduce the 3-dimensional formulation to 2-dimensional one, as also sketched in Figure 2. In the context of the corresponding weak form, this implies passing from three dimensional integration in the Cartesian coordinate system first to the integration using the cylindrical coordinates, which is then reduced to 2-dimensional integration:

$$\int_{\Omega} f(x,y,z)\mathrm{d}x\mathrm{d}y\mathrm{d}z = \int_{\Omega} \widehat{f}(r,\theta,z) r\mathrm{d}r\mathrm{d}\theta\mathrm{d}z = 2\pi \int_{S} \widehat{f}(r,z) r\mathrm{d}r\mathrm{d}z,$$

where $\widehat{f}(r,\theta,z) := f(r\cos(\theta), r\sin(\theta), z)$, and we also assumed $\Omega = S \times 2\pi$. In the following, the variables $(r,z) \in [0.25\,\mathrm{m}, 16.25\,\mathrm{m}] \times [-16\,\mathrm{m}, 0\,\mathrm{m}] =: S$ are to be re-denoted as (x,y) respectively, representing the length of S in the radial direction and the depth in the vertical direction, see Figure 2, right. Note this 'new' (x,y) are unrelated to the original 3d formulation and the coordinate notations.

The initial condition for T in S is assumed to be a positive function which decays linearly from surface to bottom:

$$T_0(x,y) := -\frac{T_{\mathrm{surf}} - T_{\mathrm{bot.}}}{H_{\mathrm{bot}}} y + T_{\mathrm{surf}},$$

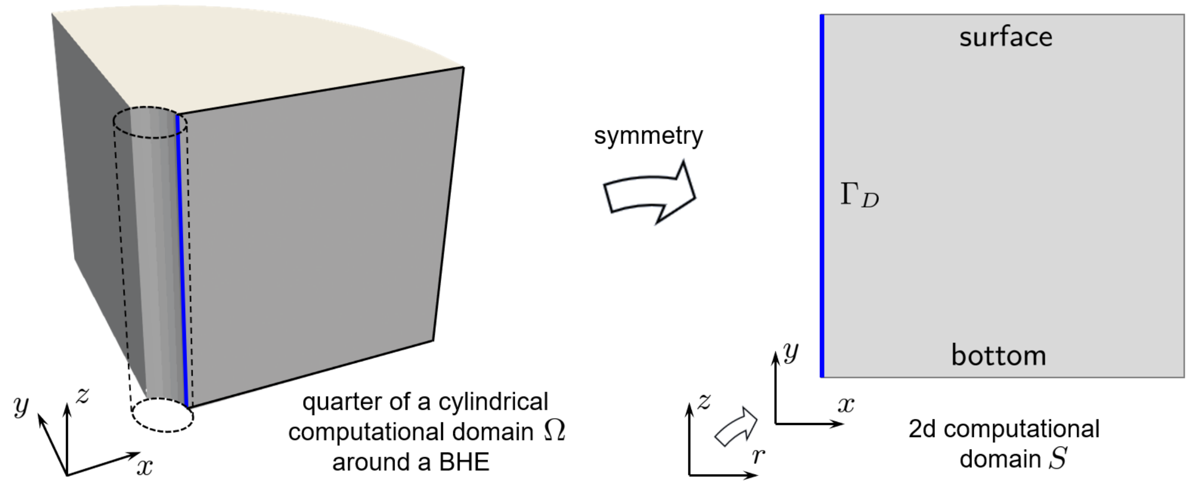


Figure 2: On the left: quarter of a cylindrical soil block around a BHE (quarter of a 3-dimensional domain Ω); on the right: reduction to 2d problem with the corresponding computational domain S, where also $(r, z) \in S$ are re-denoted as (x, y).

where $T_{\text{surf}} := 25$ °C and $T_{\text{bot}} = 10°$ C are temperature at surface and at depth of $H_{\text{bot}} = -16$ m, respectively.

For modeling the (time-dependent) boundary conditions on Γ_D of S, we assume that within the first $\widehat{t} := 10$ hours, the temperature on Γ_D drops continuously from $T_0|_{\Gamma_D}$ to the values prescribed by some continuous piece-wise linear function of y and such that at the last depth segment $y \in [H_{\text{bot}}, H_{\text{fr}}]$, where $H_{\text{fr}} := -10$ m, it becomes negative. (To recall, the latter mimics the impact of the BHE refrigerant with sub-zero temperature.) Figure 3 sketches the situation, whereas explicitly, for $t \in [0, \widehat{t}]$, we have:

$$T_1(t) := \begin{cases} -\dfrac{T_{\text{surf}} - T_{\text{bot.}}}{H_{\text{bot}}} \left(1 - \dfrac{t}{\widehat{t}}\right) y - (T_{\text{surf}} - T_{\text{fr}}) \dfrac{t}{\widehat{t}} + T_{\text{surf}}, & \text{for } y \in [H_{\text{bot}}, H_{\text{fr}}], \\ -\dfrac{T_{\text{surf}} - T_{\text{bot.}}}{H_{\text{bot}}} \left(1 - \dfrac{t}{\widehat{t}}\right) y - \dfrac{T_{\text{surf}} - T_{\text{fr}}}{H_{\text{fr}}} \dfrac{t}{\widehat{t}} y + T_{\text{surf}}, & \text{for } y \in [H_{\text{fr}}, 0], \end{cases} \tag{4}$$

where also $T_{\text{fr}} := -15$ °C. For $t > \widehat{t}$, we assume that T_1 remains fixed and is given by $T_1(\widehat{t})$ in (4). The heat conduction in the modelled case is, hence, triggered by a significant difference of temperatures on Γ_D and in S.

Finally, the material data used in our computations are depicted in Table 1.

The results of modelling are depicted in Figure 4, where we plot the temperature distribution in the soil block after 720 hours (30 days) of cooling, and also compare the outcomes of the two packages used: the OGS and the FF++. Temperature is given in kelvins. The color legend of T in the corresponding ParaView plots is tuned such that the amount of ice formed around BHEs can be identified. As expected, ice formation occurs in the vicinity of Γ_D, more specifically, near the segment of Γ_D, where the negative

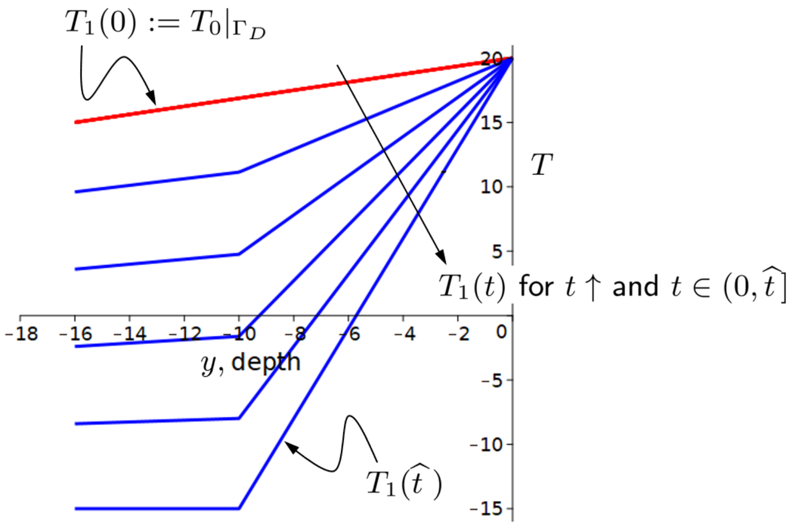


Figure 3: Temperature evolution prescribed on Γ_D within the time interval $t \in [0, \widehat{t}\,]$, where $\widehat{t} := 10$ hours; the horizontal and vertical tickmarks are in meters and °C, respectively.

solid phase	liquid phase	ice phase
$\varrho_{\rm SR} = 2000$ kg/m^3 $c_{p\rm S} = 900$ J/(kg K) $\lambda_{\rm SR} = 1.1$ W/(m K)	$\varrho_{\rm LR} = 1000$ kg/m^3 $c_{p\rm L} = 4190$ J/(kg K) $\lambda_{\rm LR} = 0.58$ W/(m K)	$\varrho_{\rm IR} = 920$ kg/m^3 $c_{p\rm I} = 2090$ J/(kg K) $\lambda_{\rm IR} = 2.2$ W/(m K) $\ell = 3.34 \cdot 10^5$ J/kg
Porosity, $\phi = 0.5$ Sigmoid function $S_{\rm I}$ coefficient, $k = 2$ Melting temperature, $T_{\rm m} = 0$ °C (273.15 K)		

Table 1: Material properties and parameters.

temperature has been prescribed. In the rest of the domain, temperature distribution remains identical to the initial condition, as can also be expected.

In either case, the P_1-based approximations of T were computed. The underlying meshes are generated with different software but in a way that the number of nodes (and elements) is comparable (almost identical). Also, each mesh is refined in a finite strip in the vicinity of Γ_D, where ice formation is expected. This is done to be able to resolve localization due to $S_{\rm I}$ and $\frac{{\rm d}S_{\rm I}}{{\rm d}T}$. The total simulation time interval is $t \in [0, 2592000\,{\rm s}] = [0\,{\rm h}, 720\,{\rm h}]$, and the time-step increment $\Delta t := 900\,{\rm s} = 15\,{\rm min}$.

In Figure 4, already the qualitative similarity of the OGS and FF++ results can be observed. Figure 5 presents the corresponding results from Figure 4 plotted over the three different (directed) lines within the domain S, thus also making the quantitative comparison feasible. For the selected lines, the compared data seems identical point-wise.

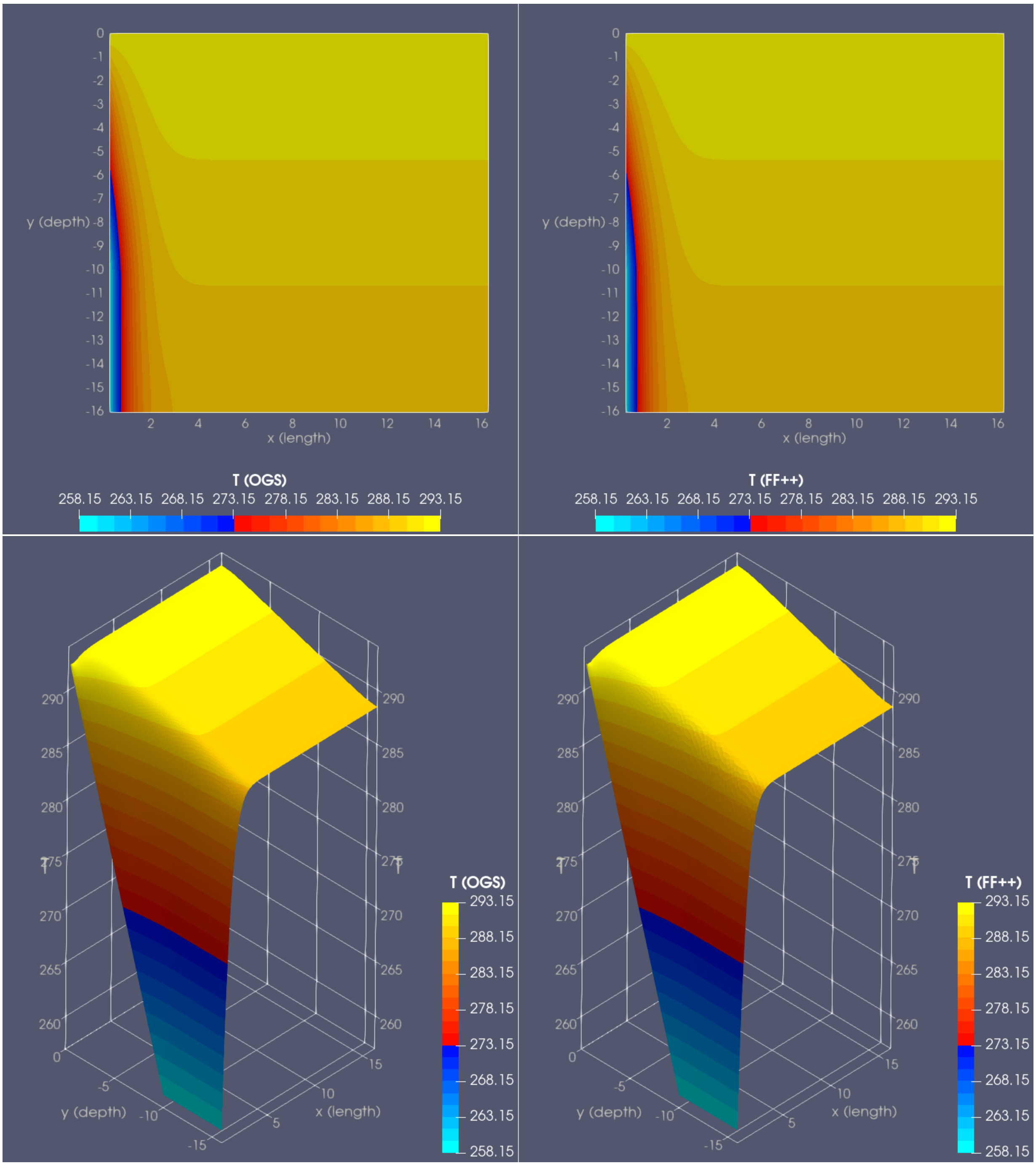
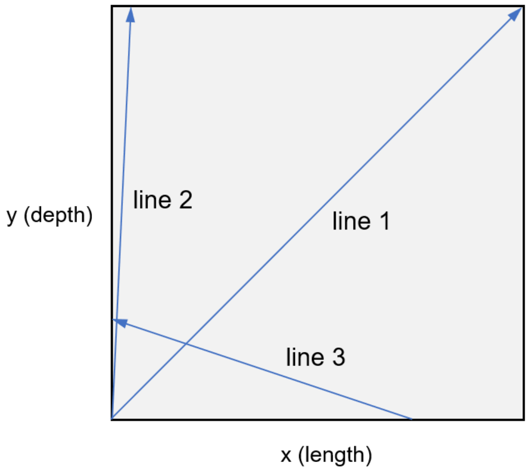


Figure 4: Comparison of the simulation results obtained by the OpenGeoSys-6 and FreeFem++ packages (in plots, termed OGS and FF++, resp.) for the setup from Figure 2: temperature T distribution within the block S after 720 hours (30 days) of cooling, 2d and 3d views; temperature is given in kelvins.



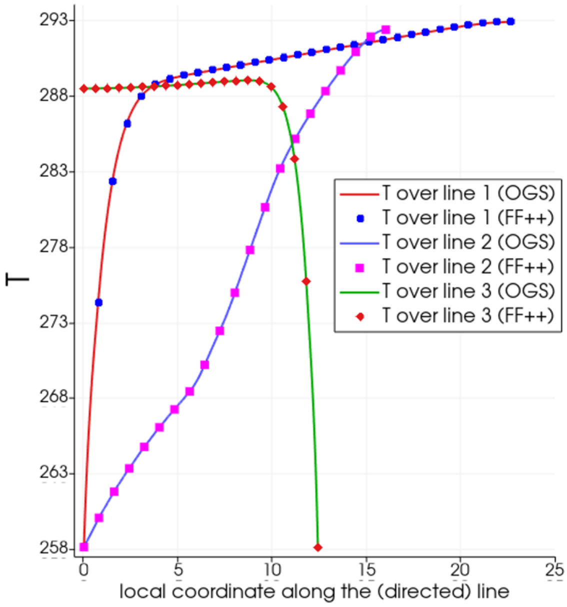


Figure 5: Comparison of the results for temperature distribution from Figure 4 over the directed lines within S; origin of the horizontal axis on the right plot corresponds to line's origin.

References

[1] F. Hecht, A. Leharic, and O. Pironneau. FreeFem++: Language for finite element method and Partial Differential Equations (PDE), Université Pierre et Marie, Laboratoire Jacques-Louis Lions, http://www.freefem.org/ff++/.