Benchmark test for the heat equation which models water-to-ice phase transition in saturated porous medium

Tymofiy Gerasimov

November 3, 2022

1 The concept of a manufactured solution

The concept of a manufactured solution can be used for code verification purposes in the case when the analytical solution of the problem of interest is not available.

To illustrate the idea, consider the boundary value problem for the Poisson equation in two dimensions:

$$\begin{cases} -\Delta u(x,y) = f(x,y) & \text{in } \Omega, \\ u = g & \text{on } \Gamma_D, \\ \frac{\partial u}{\partial \mathbf{n}} = h & \text{on } \Gamma_N, \end{cases} \tag{1}$$

where $\Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}$ is the Laplace operator, Ω is open and bounded domain, Γ_D and Γ_N are non-overlapping parts of domain's boundary $\partial\Omega$ (see Figure 1) where the Dirichlet and Neumann boundary conditions are formulated, respectively. The *direct* solution task reads: for the given data f, g, h, find the unknown u that satisfies (1).

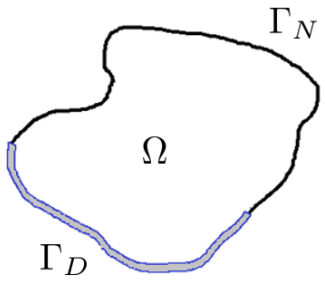

Figure 1: Sketch of the domain and its boundary partition for problem (1).

Assume the inverse situation: u is explicitly known/prescribed[1], but the right-hand

[1]and such that it is twice continuously differentiable in $\Omega \cup \partial\Omega$

sides in (1) are not. The corresponding functions f in Ω and g, h on $\partial\Omega$ can be recovered by plugging u in (1):

$$f := -\Delta u, \quad g := u|_{\Gamma_D} \quad \text{and} \quad h := \tfrac{\partial u}{\partial \mathbf{n}}|_{\Gamma_N}.$$

Note that $a|_{\Gamma_b}$ means the restriction of a to Γ_b. Such u is called a manufactured solution. If we were now to solve (1) with the u-induced right-hand sides f, g, h e.g. numerically, it would be straightforwardly to compare the computed discretization u^h – both qualitatively and quantitatively – with the already available u, thus verifying the corresponding ingredients of the numerical implementation (a code, an algorithm, a method etc.). Importantly, well-posedness of problem (1) with the given u-induced data f, g and h is guaranteed, since compatibility between these functions is automatically assured.

In the following, we apply the described approach to the initial-boundary value problem for the heat equation equation:

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

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

$$\begin{cases} T = T_0(\mathbf{x}) & \text{in } \Omega \quad \text{(IC)}, \\ T = T_1(t) & \text{on } \Gamma_D \quad \text{(BC)}. \end{cases} \tag{3}$$

Equation (2) 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 OGS documentation it is sometimes termed the "T+freezing" equation.

In (2), 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,

$$S_{\text{I}}(T) := \frac{1}{1 + e^{k(T - T_{\text{m}})}}, \quad k > 1, \; T_{\text{m}} = 273.15\,\text{K}, \tag{4}$$

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 2.

Also in (2), parameter ℓ is the so-called heat of fusion of ice, whereas all other parameters in (2) are standard ones related to the classical THM modeling of processes in saturated porous medium.

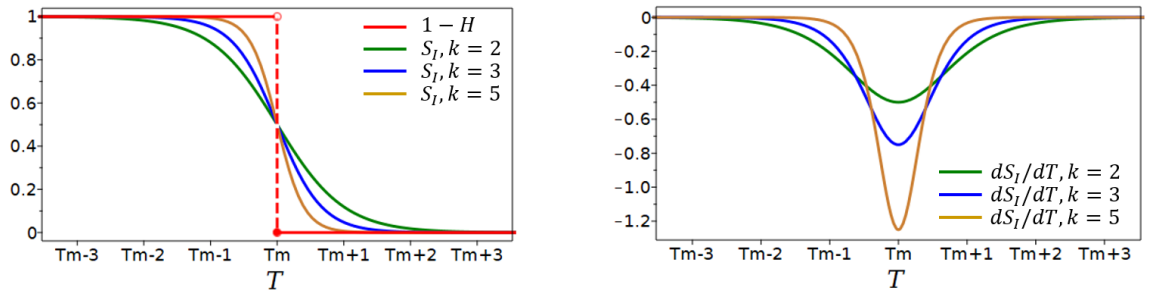

Figure 2: On the left: plots of the Heaviside-like ice-fraction indicator function (denoted as $1-H$) and its regularized counterpart S_{I}; on the right: plots of the first-order derivative of S_{I}.

2 Simulation of the ice melting-forming process

In this benchmark example, we restrict ourselves to 2-dimensional formulation (2)-(3) in $\Omega := (0,1)^2$. We also opt for dealing with only the Dirichlet type boundary data, that is, $\Gamma_D := \partial\Omega$ is assumed. The manufactured $T = T(x,y,t)$ with $t \in (0,1]$ is chosen in such a way that its evolution in time mimics the **simultaneous ice melting-forming process**. We will bring the expressions for Q_T, T_0 and T_1 required in (2)-(3) explicitly. Our OpenGeoSys-6 implementation is tested when Ω is discretized by bi-linear quadrilaterals such that the corresponding FE solution T^h at any fixed time step is in Q^1-spaces. Finally, the material data and parameters in (2) used in the numerical experiment are depicted in Table 1.

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

Table 1: Material properties and parameters.

Our manufactured solution T for (2)-(3) is given by

$$T(x,y,t) := b\left[xy\cos\left(\frac{1}{2}\pi t\right) + (1-x)y\sin\left(\frac{1}{2}\pi t\right)\right] + c, \tag{5}$$

where $(b,c) = (17, -7 + 273.15)$. The snapshots of T measured in degrees Celsius are depicted in Figure 3. Again, from the physics standpoint the evolution of temperature

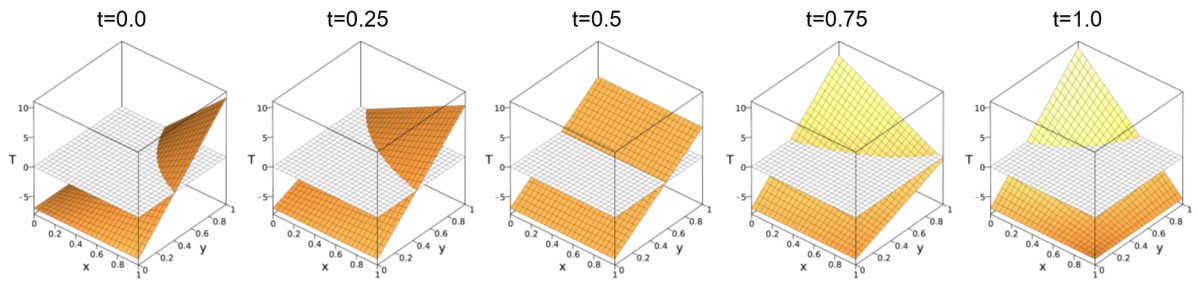

Figure 3: Snapshots of T given by (5) in degrees Celsius. The plane in white color represents zero (melting) temperature $T_{\mathrm{m}} = 0^{\circ}$ C; hence, the zero-level set of T mimics the interface between ice and water fractions which moves in time.

defined by such T mimics both ice formation and ice melting within the domain which is initially partly occupied by ice and liquid.

Using (5), the right-hand side data for (2)-(3) is recovered. The source term Q_T in Ω reads:

$$Q_T := \left((\varrho c_p)^{\mathrm{eff}} - \ell \varrho_{\mathrm{IR}} \frac{d\phi_{\mathrm{I}}}{dT}\right) \frac{1}{2}\pi b y \left[(1-x)\cos\left(\frac{1}{2}\pi t\right) - x \sin\left(\frac{1}{2}\pi t\right)\right]$$

$$-(\lambda_{\mathrm{IR}} - \lambda_{\mathrm{LR}}) \frac{d\phi_{\mathrm{I}}}{dT} b^2 \left[y^2(1-\sin(\pi t)) + x(1-x)\sin(\pi t) + \left(x - \frac{1}{2}\right)\cos(\pi t) + x^2 - x + \frac{1}{2}\right]. \tag{6}$$

The initial condition function T_0 in Ω is as follows:

$$T_0(x,y) := T(x,y,0) = bxy + c.$$

Finally, assuming Γ_D to be composed of all four sides of the unit square, the boundary condition function T_1 is also obtained:

$$T_1(t) := \begin{cases} c, & \text{on } \{x \in (0,1), y = 0\}, \\ by\cos\left(\frac{1}{2}\pi t\right) + c, & \text{on } \{x = 1, y \in (0,1)\}, \\ b\left[x\cos\left(\frac{1}{2}\pi t\right) + (1-x)\sin\left(\frac{1}{2}\pi t\right)\right] + c, & \text{on } \{x \in (0,1), y = 1\}, \\ by\sin\left(\frac{1}{2}\pi t\right) + c, & \text{on } \{x = 0, y \in (0,1)\}. \end{cases}$$

Figure 4 depicts comparison of the snapshots of T given by (5) and the solution T^h to (2)-(3) obtained with the OGS. The temperature given in Kelvins. Note that we have made the vertical range of the OGS solutions in the Paraview plots 10^{-1} rescaled, to make the comparison feasible. Also, we have tuned the color legend in the Paraview plots such that the ice and water fractions can be visible/identified.

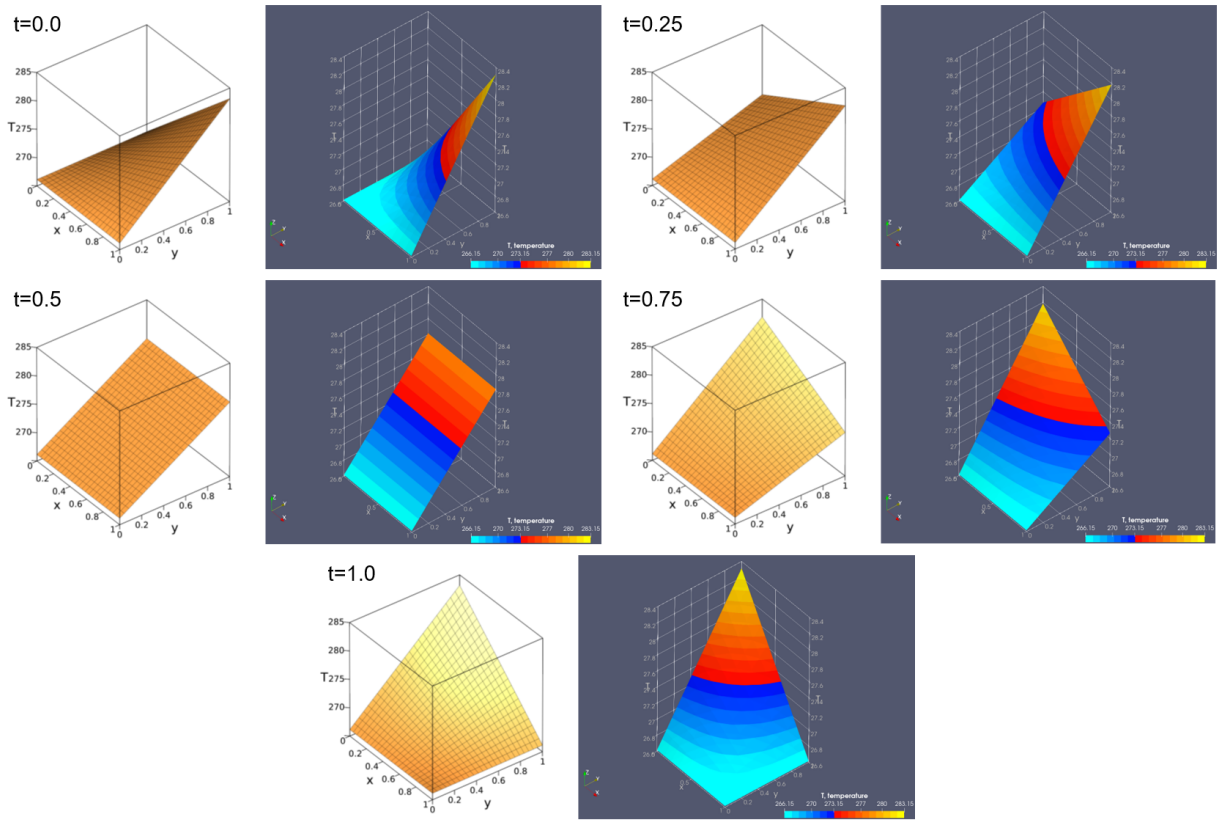

Figure 4: Comparison of manufactured solution (left) with the numerical one (right) computed by the OGS at different time steps; temperature is given in degrees Kelvin.