NUMERICAL SIMULATION OF THE HEAT TRANSPORT AND FLOW PROBLEMS WITH PHASE CHANGE

{ Valentin Alekseev & Maria Vasilyeva}   North-Eastern Federal University, Yakutsk, Russia

Introduction

In this work, we consider the numerical solution of a heat transfer and flow problems in homogeneous domains with phase change. Mathematical model contains convection-diffusion equation for the temperature and Stokes or Darcy equation for the flow. Heat transfer with phase change described by the Stefan model. For simulation of flow with moving phase change boundary, we use fictitious domain method.
The main difficulty in solving such problems is related with the convection-diffusion equation in the case when convective term dominates over diffusion. The standard approximation using the classical Galerkin method can lead to oscillations in the solution of the problem. In this work we use the SUPG (streamline upwind Petrov-Galerkin) method. For approximation of flow problem, we use Taylor-Hood finite elements for Stokes flow and mixed finite element method for Darcy flow.
We present the numerical results for model problem in domain with inclusions in two-dimensional and three-dimensional formulations.

Heat and mass transfer

In this section, we consider a non-stationary convection-diffusion equation that describes the transfer of heat in homogeneous domains:

$$\frac{\partial T}{\partial t} + u\nabla T - \operatorname{div}(d\nabla T) = 0. \tag{1}$$

where d is a diffusive transfer coefficient.
The flow velocity is determined by the Stokes equation, which is used to describe the flow at the micro level:

$$\begin{cases} -\mu\Delta u + \nabla p = 0, \\ \operatorname{div} u = 0. \end{cases} \tag{2}$$

where μ is a viscosity
The equations (1)-(2) is supplemented by corresponding initial and boundary conditions.

Finite-element approximation for SUPG method

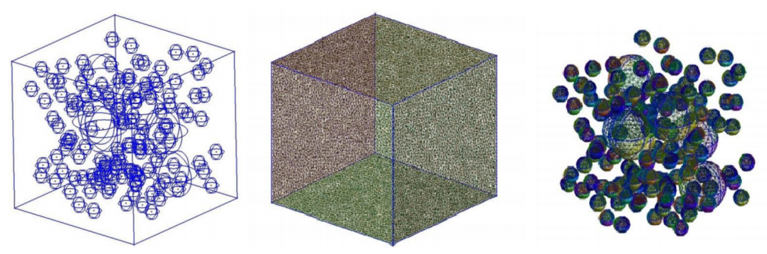
It is known that the approximation of the convection-diffusion equations using the standard Galerkin method leads to oscillations in the solution of the problem and is not suitable for calculations in the case of dominance of a convective term over a diffusion one. Therefore, we use the method of the SUPG. The main idea of SUPG is the modification of the test functions taking into account the direction of the flow. In the SUPG method, the following variational formulation is used for the equation (1): find $T^{n+1} \in Q$ $(n = 1, 2, \dots)$ such that

$$\int_\Omega \frac{T^{n+1} - T^n}{\tau}\overline{r}dx - \int_\Omega \left(d\nabla T^{n+1}, \nabla\overline{r}\right) + \int_\Omega u\nabla T^{n+1}\overline{r}dx = 0, \quad \forall v \in Q,$$

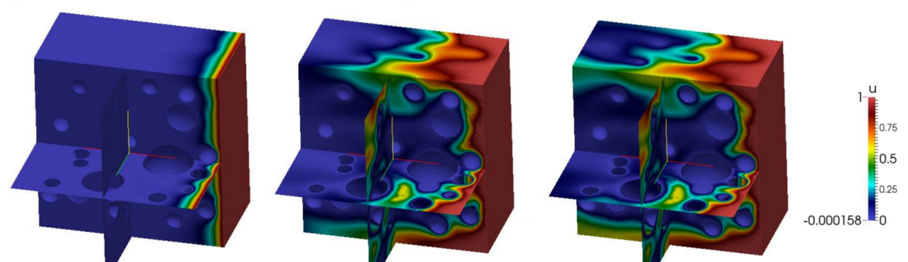
where $\forall \overline{r} \in \overline{Q}, \overline{r} = \left(r + \frac{h}{2|u|}u\nabla r\right)$.

3D results

Here we consider three dimensional heat transfer problem without phase change. We consider temperature distribution in the domains with inclusions. The computational domain consists of a random number of inclusions with random size. Initial temperature is $T_0 = 0°C$. For numerical simulations, we set Dirichlet boundary conditions: in right boundary $T = 1°C$, in all boundary $u = 1$.



Computational domain and computational mesh with 1016931 elements.



Temperature distribution at t=0.05, t=0.75, t=1.5, respectively.

	t
1	2325
2	1299.4
4	777.4
8	555.8
16	381.1

Execution time in sec.(left:Number of processors)

Stefan model and Stokes flow

For simulation of heat transfer processes with phase change, we use a classic Stefan model

$$\left(\alpha(\phi) + \rho^+ L\phi'\right)\left(\frac{\partial T}{\partial t} + ugradT\right) - \operatorname{div}\left(\lambda(\phi)\operatorname{grad} T\right) = 0,$$

where L is a specific heat of the phase change For the coefficients we have the following relationships of heat capacity and thermal conductivity:

$$\alpha(\phi) = c_i\rho_i + \phi(c_w\rho_w - c_w\rho_w), \quad \lambda(\phi) = \lambda_i + \phi(\lambda_w - \lambda_i),$$

The indexes w, i denote the water and ice, respectively. In practice, the phase transitions occur in a small temperature range $[T^* - \Delta, T^* + \Delta]$. As the function ϕ we take ϕ_Δ:

$$\phi_\Delta = \begin{cases} 0, & T \le T^* - \Delta, \\ \dfrac{T - T^* + \Delta}{2\Delta}, & T^* - \Delta < T < T^* + \Delta, \\ 1, & T \ge T^* + \Delta, \end{cases}$$

Therefore, we get the following equation for nonlinear parabolic temperature in the domain Ω:

$$\left(\alpha(\phi_\Delta) + \rho_l L\phi'_\Delta\right)\left(\frac{\partial T}{\partial t} + ugradT\right) - \operatorname{div}(\lambda(\phi_\Delta)\operatorname{grad} T) = 0. \tag{3}$$

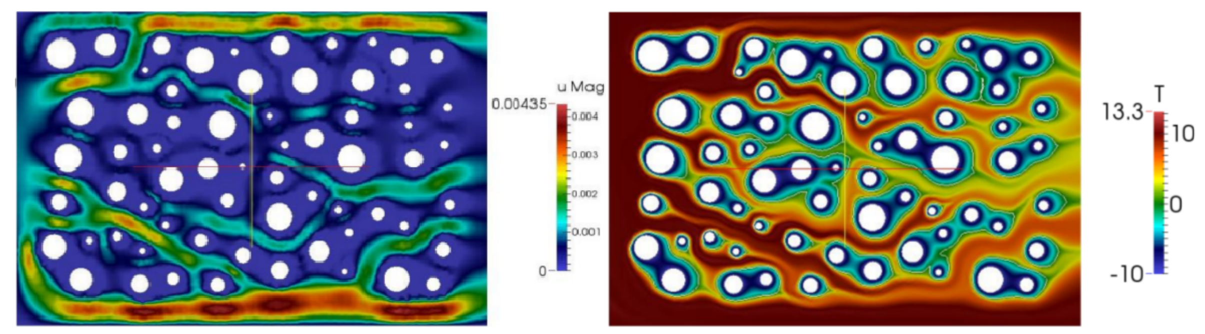
The flow velocity is determined by the Stokes equations:

$$\begin{cases} -\mu\Delta u + \nabla p = 0 + Au, \\ \operatorname{div} u = 0. \end{cases} \tag{4}$$

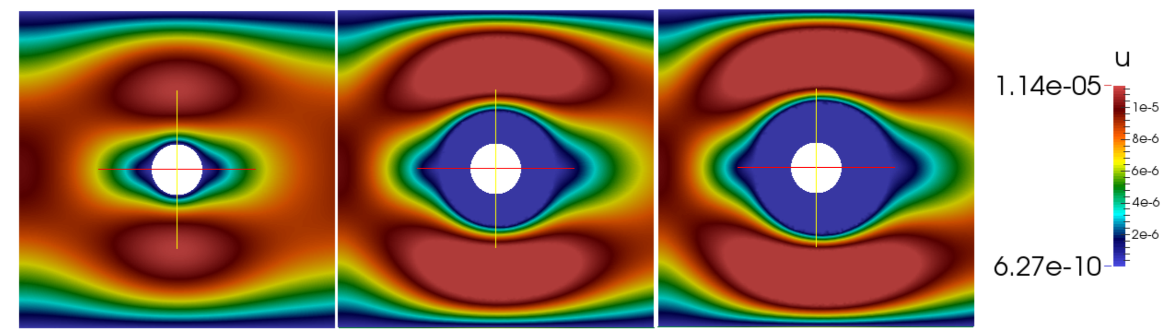
where μ is a viscosity, A is defined so that momentum equations are forced to mimic the Carman-Kozeny equations

$$A = -C\frac{(1-\epsilon)^2}{\epsilon^3 + b}$$

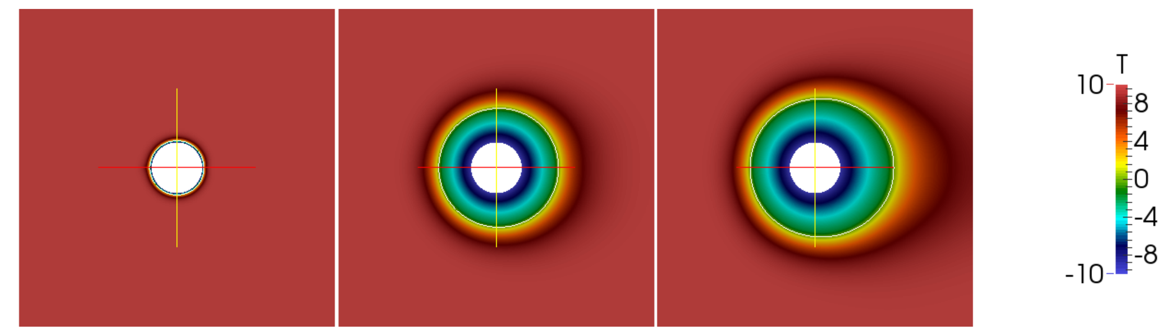
where C is a constant accounting for the mushy-region morphology, ϵ is the porosity between 0 and 1 and $b = 10^{-6}$ is a constant introduced to avoid division by zero. The equation (3)-(4) is supplemented by corresponding initial and boundary conditions. We consider temperature, velocity distributions in the soils with permafrost for phase change case. Inclusion simulate freezing columns, where we set constant low temperature.Initial temperature is $T_0 = 10°C$. We assume that the phase transition temperature is $T^* = 0°C$. For numerical simulations, we set Dirichlet boundary conditions: in inclusion $T = -10°C$; in left boundary $u = 0.00001$.



Model 2:Velocity(left) and temperature(right) distribution at t=1sec., t=25sec., respectively.



Model 1:Velocity distribution at t=1sec., t=15sec., t=30sec., respectively.



Model 1:Temperature distribution at t=1sec., t=15sec., t=30sec., respectively.

Stefan model and Darcy flow

For simulation of heat transfer processes with phase change, we use a classic Stefan model

$$\left(\alpha(\phi) + \rho^+ L\phi'\right)\left(\frac{\partial T}{\partial t} + ugradT\right) - \operatorname{div}\left(\lambda(\phi)\operatorname{grad} T\right) = 0,$$

where L is a specific heat of the phase change, m is a porosity, ρ^+, c^+, λ^+ and ρ^-, c^-, λ^- are density, specific heat capacity and thermal conductivity of melted and frozen zones, respectively. We have the following coefficients

$$\alpha(\phi) = c^-\rho^- + \phi(c^+\rho^+ - c^-\rho^-), \quad \lambda(\phi) = \lambda^- + \phi(\lambda^+ - \lambda^-),$$

$$c^-\rho^- = (1-m)c_{sc}\rho_{sc} + mc_i\rho_i, \quad \lambda^- = (1-m)\lambda_{sc} + m\lambda_i,$$

$$c^+\rho^+ = (1-m)c_{sc}\rho_{sc} + mc_w\rho_w, \quad \lambda^+ = (1-m)\lambda_{sc} + m\lambda_w.$$

and

$$\phi = \begin{cases} 0, & \text{when } T < T^*, \\ 1, & \text{when } T > T^*, \end{cases}.$$

The indexes sc, w, i denote the solid skeleton, water, and ice, respectively. In practice, the phase transitions occur in a small temperature range $[T^* - \Delta, T^* + \Delta]$. As the function ϕ we take ϕ_Δ:

$$\phi_\Delta = \begin{cases} 0, & T \le T^* - \Delta, \\ \dfrac{T - T^* + \Delta}{2\Delta}, & T^* - \Delta < T < T^* + \Delta, \\ 1, & T \ge T^* + \Delta, \end{cases}$$

Therefore, we get the following equation for nonlinear parabolic temperature in the domain Ω:

$$\left(\alpha(\phi_\Delta) + \rho_l L\phi'_\Delta\right)\left(\frac{\partial T}{\partial t} + ugradT\right) - \operatorname{div}(\lambda(\phi_\Delta)\operatorname{grad} T) = 0. \tag{5}$$

The flow velocity is determined by the Darcy equations:

$$\begin{cases} -u + \frac{k}{\mu}(gradp) = 0, x \in \Omega \\ \operatorname{div} u = 0. \end{cases} \tag{6}$$

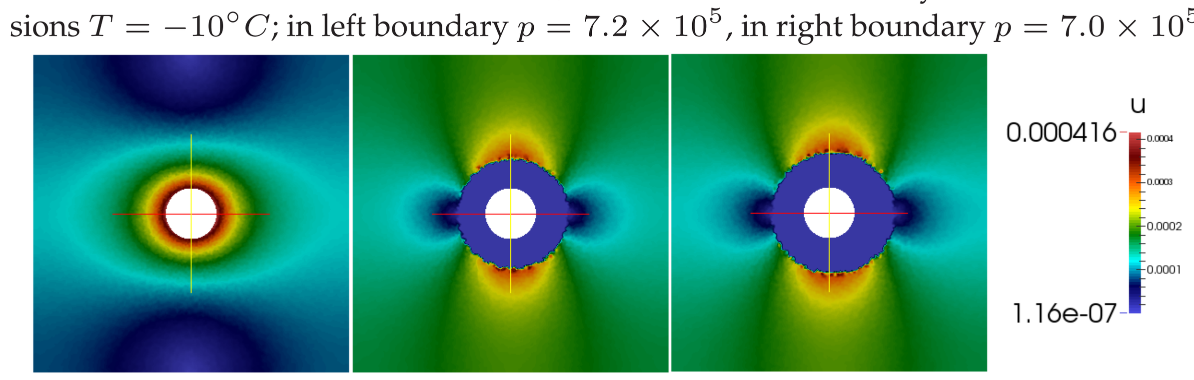
where μ is a viscosity k is a tensor of absolute permeability of a porous medium.
The problems of calculating the system of the Darcy flow equation are generated, first of all, by the fact that the problem 6 is a problem with a moving boundary S. To solve this problem numerically without rebuilding the computational grid, we use the method of fictitious domains, which is based on the transition to the solution of the problem in a wider area. An approximate solution depending on the continuation parameter ϵ will be searched throughout the calculation domain Ω. When using the method of fictitious domains with a continuation with respect to the highest coefficients, the solution is determined from equation.

$$-u + \theta_\epsilon(gradp) = 0, x \in \Omega$$

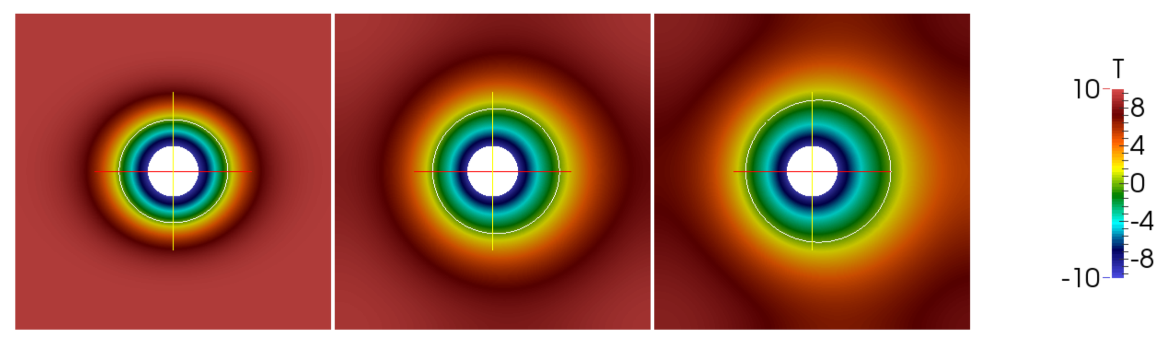
where $\theta_\epsilon(x)$ is a discontinuous coefficient which is define by expression

$$\theta_\epsilon(x) = \begin{cases} \frac{k}{\mu}, & x \in \Omega^+ \\ \epsilon^2, & x \in \Omega^- \end{cases}.$$

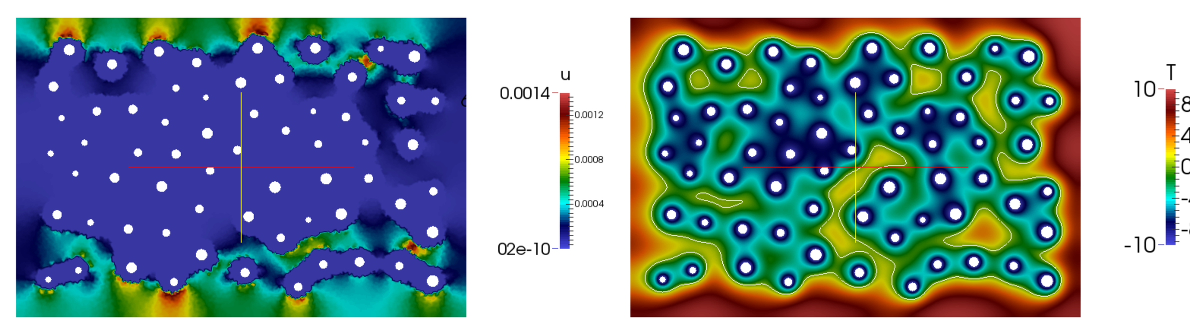
with sufficient small ϵ.
The equation (5)-(6) is supplemented by corresponding initial and boundary conditions. We present numerical results. We consider temperature distribution in the soils with permafrost for phase change case. Inclusion simulate freezing columns, where we set constant low temperature.
Initial temperature is $T_0 = 10°C$. We assume that the phase transition temperature is $T^* = 0°C$. For numerical simulations, we set Dirichlet boundary conditions: in inclusions $T = -10°C$; in left boundary $p = 7.2 \times 10^5$, in right boundary $p = 7.0 \times 10^5$



Model 1:Velocity distribution at t=1sec., t=75sec., t=150sec., respectively.



Model 1:Temperature distribution at t=1sec., t=75sec., t=150sec., respectively.



Model 2:Velocity(left) and temperature(right) distribution at t=1sec., t=50sec., respectively.

Conclusion and future works

In this work we have considered the problems of heat and mass transfer in homogeneous domains, and we have studied the problems with a phase change. For numerical solutions of the convective-diffusive heat transfer, we used the approximation schemes with numerical stabilization for finite element methods. For mass transfer, we used a Stokes and Darcy equations for the flow. Heat transfer with phase change described by the Stefan model. For simulation of flow with moving phase change boundary, we used fictitious domain method.For approximation of flow problem, we used Taylor-Hood finite elements for Stokes flow and mixed finite element method for Darcy flow.
We showed the numerical results for Darcy and Stokes flow for different geometries for two-dimensional and three-dimensional formulation.
Future works:

- Construct multiscale model reduction for the stokes flow in perforated domains using GMsFEM
- Construct multiscale basis for the heat transfer using mixed formulations
- Multiscale model reduction for heat and mass transfer with phase change

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Contact Information

Email alekseev.valen@mail.ru