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Numerical modeling of non-stationary heat problems in a two-phase medium

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Abstract. The simulation of thermal fields and melting permafrost is an important step for engineering construction in many regions of Russia. Water-ice phase transitions in a 3-D complicated computation domain must be taken into account. The enthalpy statement with an implicit finite volume method was used to create a good discretization and a local mesh refinement to focus an area near the oil well. System of linear algebraic equations is solved using the iterative conjugate residual or conjugate gradient method in Krylov subspaces with the incomplete factorization algorithm in the Eisenstat modification as a preconditioner. A special high-parallel version of matrix generation and solving a system of the linear algebraic equations code have been developed and then efficiency has been estimated. The performance results of the developed code and temperature fields for different wells configuration (1 well and 4 wells placed as squared) during 5 years have been presented. The results validation was based on the comparison with previous papers and other algorithms. The results of simulations are close those to presented by other authors.

1. Introduction

The oil production in northern conditions requires the prediction of heating permafrost around wells and engineering structures. The simulation of thermal fields should take into account the complicated 3D geometry with contrasting material properties, water-ice phase transitions and seasonal changes in the temperature of a medium. This problem has been focused by many authors, see [1] - [6] but developing efficient high-parallel algorithm for a modern high performance computation system with real input data to predict thermal fields in permafrost still remains open.

We can use the enthalpy approach because we do not need to calculate the exact boundaries of the phase transition, which is optional for the problem to be solved. The key issues of modeling the thermal field near the wells are the following: the first is a different scale of the objects, since the diameter of the well is usually about 20 centimeters, while the heating effects of a region are measured as hundreds of meters; the second is the prediction during many years; the third is the dependence of the model coefficients on temperature, which makes the problem non-linear; and the last one is temperature on soil with allowance seasons conditions. The stable implicit Crank-Nikolson finite volume schemes with respect to time [7] - [10] are used. Iterative sparse solver has been adapted at each step to problem features. To solve complex thermal



field modeling problem, we have to develop an efficient parallel algorithm and to provide code optimizations for Intel Xeon Phi many-core hardware architecture.

A regular tetragonal mesh with local refinement was created to resolve the object size imbalance between the domain size and the well diameter. This approximation has the first order in time and space and requires a special type of the representation enthalpy. The resulting system of linear algebraic equations is solved using the iterative conjugate residual (CR, Conjugate Residual) or conjugate gradient (CG, Conjugate Gradient) method in the Krylov subspaces using the incomplete factorization algorithm in the Eisenstat modification as a preconditioner. Choosing the advanced initial guess for solving SLAEs helps to decrease the number of iterations for each time step [11]. We take into account a general surface condition model which includes seasonal changes in temperature.

The paper is organized as follows. Section 2 deals with to the problem statement, which describes the heat equations and a difference between approach proposed and standard one. Section 3 describes approximation methods in detail. Section 4 presents the mathematical background to adapt an iterative solver and to find a good initial guess for time steps. Section 5 provides the details of computational experiments and results obtained. The last section summarizes, gives the conclusion and discussion of further research.

2. Problem Statement

Let us consider the initial boundary value problem in the computational domain $\Omega \times t$, $\Omega \in R^3$, $t \in R^1$ with a piecewise smooth boundary Γ of Ω . We assume that the phase state changes at a constant predetermined temperature $T = T^*$. By $S(t)$ we denote the interface between two phases of media, i.e. a medium with ice (denote by $\Omega^+(t) = \{(x, y, z) \mid (x, y, z) \in \Omega, T(x, y, z, t) > T^*\}$) and a medium with water (we denote by $\Omega^-(t) = \{(x, y, z) \mid (x, y, z) \in \Omega, T(x, y, z, t) < T^*\}$). The enthalpy setting given in [1] was used:

$$\frac{\partial H}{\partial t} + u * \text{grad}(H) - \text{div}(\lambda * \text{grad}(T)) = 0, \quad (1)$$

where $H(x, t)$ is the enthalpy, λ is the thermal conductivity and u is the flow velocity vector in a porous medium, which, in our case, is equal to zero. Enthalpy is a function of temperature $T(x, y, z, t)$ and the ice coefficient ψ , which determines the proportion of ice/water in volume:

$$\psi = \begin{cases} 0, & T < T^*, \\ \in [0, 1], & T = T^*, \\ 1, & T > T^*, \end{cases} \quad (2)$$

such that $H(T, \psi) = \rho c T + \rho L \psi$, L is the phase transition heat, c is the mass heat capacity and ρ is the material density. We consider the phase transition defined in the neighborhood size Δ of T^* , as was presented in [2] or use the following modified enthalpy $\bar{H}(T^* - \Delta) = H(T^* - \Delta) = \rho^- c^- (T^* - \Delta)$, $\bar{H}(T^* + \Delta) = H(T^* + \Delta) = \rho^+ c^+ (T^* + \Delta) + L$, where c^- , ρ^- and c^+ , ρ^+ are mass the heat capacity and the material density in Ω^- and Ω^+ and we are able to define any reasonable $\bar{H}(T)$ for $T \in [T^* - \Delta, T^* + \Delta]$ satisfying equations presented before. Then we obtain the following statement:

$$(C_\Delta + \rho^+ L \psi_\Delta) \frac{\partial T}{\partial t} - \text{div}(\lambda_\Delta * \text{grad}(T)) = 0, \quad (3)$$

$$C_\Delta = \begin{cases} \rho^- c^-, & T \leq T^* - \Delta, \\ \rho^- c^- + (\rho^+ c^+ - \rho^- c^-) * \frac{T - T^* + \Delta}{2\Delta}, & T^* - \Delta < T < T^* + \Delta, \\ \rho^+ c^+, & T \geq T^* + \Delta, \end{cases} \quad (4)$$

$$\psi_{\Delta} = \begin{cases} 0, & T \leq T^* - \Delta, \\ \frac{1}{2\Delta}, & T^* - \Delta < T < T^* + \Delta, \\ 0, & T \geq T^* + \Delta. \end{cases} \quad (5)$$

$$\lambda_{\Delta} = \begin{cases} \lambda^-, & T \leq T^* - \Delta, \\ \lambda^- + (\lambda^+ - \lambda^-) * \frac{T - T^* + \Delta}{2\Delta}, & T^* - \Delta < T < T^* + \Delta, \\ \lambda^+, & T \geq T^* + \Delta, \end{cases} \quad (6)$$

where λ^- and λ^+ are thermal conductivities in Ω^- and Ω^+ . To use the approximation of the thermal conductivity coefficient taking into account the phase transition comes from the previous time step and constructing a first-order finite volume scheme with respects to time, it is necessary to use the continuous enthalpy function together with its first derivative, which leads to the following modification of the formulation [5] and the use of $\bar{\psi}_{\Delta}$ instead of ψ_{Δ} :

$$(C_{\Delta} + \rho^+ L \bar{\psi}_{\Delta}) \frac{\partial T}{\partial t} - \text{div}(\lambda_{\Delta} * \text{grad}(T)) = 0, \quad (7)$$

$$\bar{\psi}_{\Delta} = \begin{cases} 0, & T \leq T^* - \Delta, \\ \frac{T - (T^* - \Delta)}{\Delta^2}, & T^* \leq T \leq T^* + \Delta, \\ \frac{1}{2\Delta} - \frac{T - (T^* - \Delta)}{\Delta^2}, & T^* - \Delta \leq T \leq T^* + \Delta, \\ 0, & T \geq T^* + \Delta, \end{cases} \quad (8)$$

and the coefficients ρ^+ , ρ^- , c^+ , c^- , λ^+ and λ^- in (3)-(8) are determined, as presented in [3]: For simplicity, we construct the enthalpy functions (see Figure 1) for the case with a certain fixed set of coefficients. As can be seen from Figure 1 for a different kind of ice coefficient, we have a jump in the enthalpy function at the point T^* for ψ , the jump in the first derivative of enthalpies at the points $T^* \pm \Delta$ for ψ_{Δ} and a continuous function of the enthalpy itself and its first derivative for $\bar{\psi}_{\Delta}$. We supplement these statements with initial and boundary conditions. The initial condition for the temperature distribution in the domain Ω is written down as

$$T|_{t=0} = T_0(x, y, z). \quad (9)$$

At the outer boundary Γ of the computational domain, which we take far remover from wells, the following boundary conditions of the first kind are set (the Dirichlet condition, the given temperature T_d) or boundary conditions of the 2-nd kind (the Neumann condition, the given heat flux, J_n):

$$T|_{\Gamma_D} = T_d(x, y, z, t), \quad (10)$$

$$\lambda \frac{\partial T}{\partial n}|_{\Gamma_N} = J_n(x, y, z, t), \quad (11)$$

where $\Gamma = \Gamma_D \cup \Gamma_N$.

3. Discretization and Approximation of the Initial Boundary Value Problem

A regular tetragonal mesh with a local refinement was created to resolve the object size imbalance between computational domain size and well diameters. For the case with one well, we use a single-level mesh refinement; for the case with four wells located in a parallelepiped, the two-level mesh concentration is used as is shown in Figure 2. The initial boundary value problem (3)-(11) is approximated in the computational domain Ω , and $0 < t < t_e$ with respect to time using the implicit Crank-Nicolson scheme [6], and with respect to space using the finite volume method on the quasi-structured grid [7, 8], obtained with integral conservation laws taking into account the initial and boundary conditions (9)-(11), on an adaptive unstructured grid [9]. In this case, adaptability is understood to mean that all the angular points of the

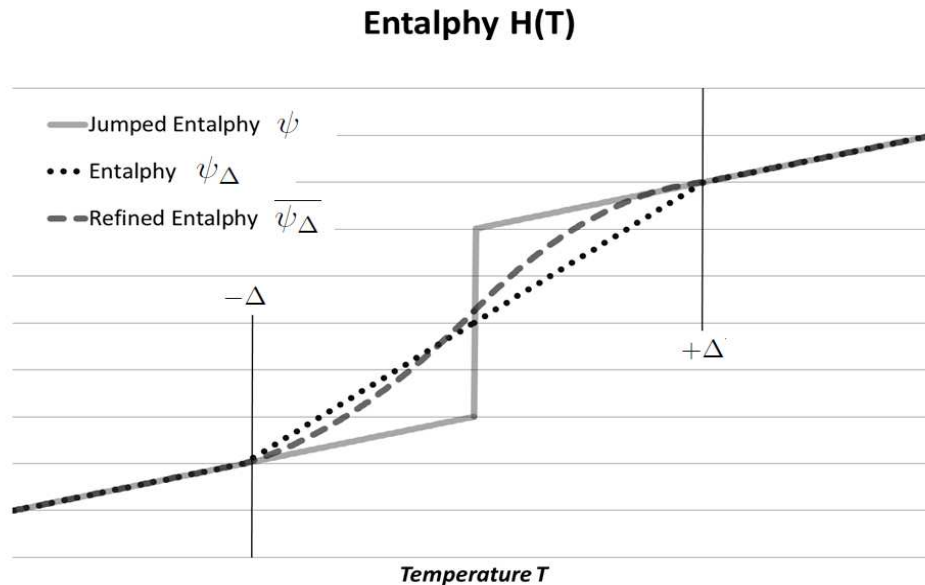


Figure 1. The enthalpy function noted as Jumped Enthalpy in the case ψ ; Enthalpy in the case ψ_Δ and Refined Enthalpy for ψ_Δ

external and internal boundaries are grid nodes. In approximating the initial boundary value problem (1), (4), (7), (8), (9)–(11) we assume only the existence of its classical solution at all internal points $(x, y, z) \in \Omega$, which is sufficiently piecewise smooth up to the external border. The thermal conductivity coefficient taking into account the phase transition was explicitly calculated at the centers of finite elements according to the values of the temperature field from the previous time step. This approximation has the first order with respect to time and space, which was confirmed by a number of model problems with a well-known analytical solution, on a sequence of condensing grids.

The finite volume methods (FVM) are used to approximate the problem coming from integral conservation laws taking into account the boundary conditions and relations at internal boundaries. As basis functions, we use the piecewise linear tetrahedron elements, so approximation is made on an adaptive tetrahedral unstructured grid. Denoting by Γ_l the boundary of the finite volume V_l and integrating equation (1) over time and space, we obtain the following integral form of the conservation law:

$$\int_{V_l} c (T^{n+1} - T^n) dv = \int_{t_n}^{t_{n+1}} \int_{\Gamma_l} \frac{\partial T}{\partial n} ds dt \quad (12)$$

where T^{n+1} and T^n are the temperatures for t_{n+1} and t_n time steps. Let us consider local matrices for the FVM and we can separately approximate each of the integrals given in equation (12) as is presented in [7]. The element-by-element technology was used for an assembly of global matrix in parallel. We give attention to choosing an effective approach to organizing a parallel matrix assembly. As options, let us consider two options: the node-based and the element-base of parallel assembling of a matrix. Element-base approach means computing a local matrix for each entry only once and accumulation global matrix as the sum of thread matrices with synchronization overhead, because many global matrix rows partially computed by different threads, see Figure 3. The node-based approach is based on computation of a full row in a thread, but it may require computing the local matrix of one grid element several times - by the number of nodes of an element belonging to different threads, but accumulating

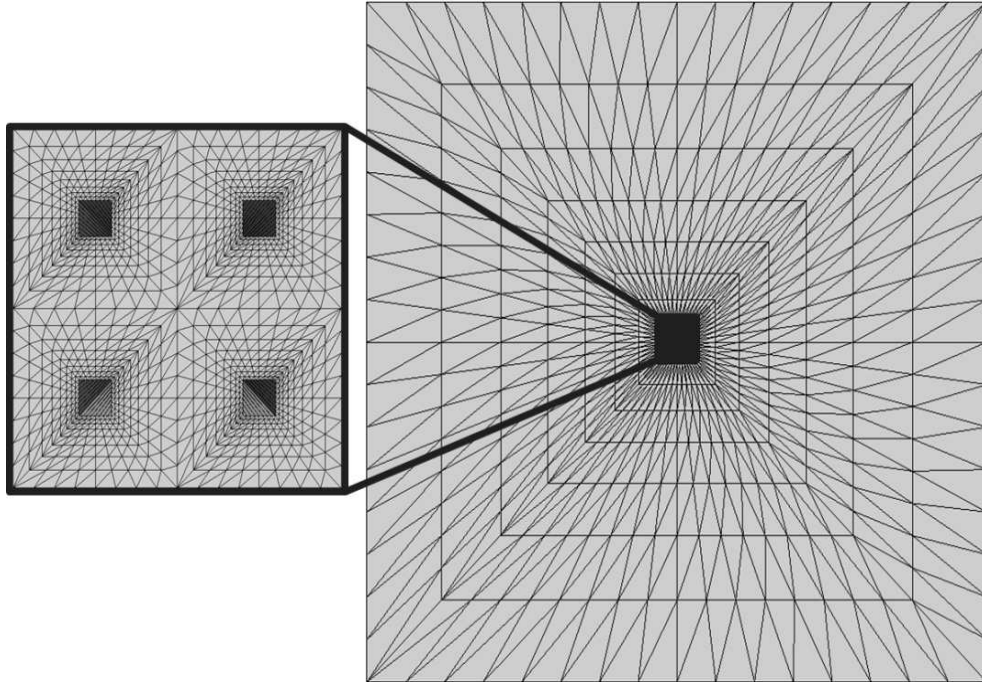


Figure 2. The two-level regular mesh concentration in the three-dimensional domain for the case with 4 shafts (from the top).

the global matrix does not require an extra effort (see Figure 4). We estimate the times based on the roof-line model [12] and the node-based parallel algorithm looks better for many-core architecture like Xeon Phi.

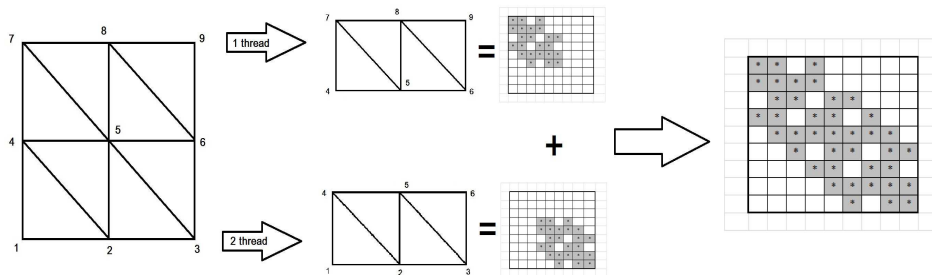


Figure 3. The element-based approach taking much time to thread assembling global matrix.

To solve the resulting system, the KRYLOV iterative sparse solvers library [13], to accelerate special choice of the initial guess was used and described in detail below.

4. Choosing the Initial Guess for solving SLAEs

One important issue in solving a non-stationary problem consists in choosing the initial guess for the iterative solution of SLAEs at each time step. It is natural that the temperature T^n denoted as u^n would be a good approximation to u^{n+1} to reduce the number of iterations, provided that the time step $\tau_n = t_n - t_{n-1}$ is sufficiently small. Another simple approach is based on the linear extrapolation with respect to time [11]:

$$u^{n+1} = u^n + (u^n - u^{n-1})\tau_n/\tau_{n-1} + O(\tau^2).$$

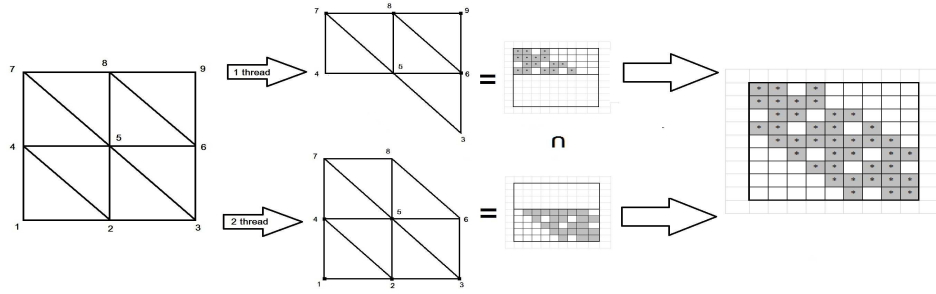


Figure 4. The node-based approach takes a greater number of operations to calculate more local matrices.

In this case, we need to save the numerical solution for one additional time step. One of the popular methods for solving ODEs is based on the application of predictor-corrector schemes. For example, if we use in the Crank-Nicolson scheme [8], written as

$$\begin{aligned} Cu^{n+1} &\equiv (\tau_n^{-1}B + \theta A)u^{n+1} = g^{n+1}, \\ g^{n+1} &= [\tau_n^{-1}B + (1 - \theta)A]u^n + \theta f^{n+1} + (1 - \theta)f^n, \end{aligned} \quad (13)$$

where A is the space approximation of the differential operator, $\psi^\tau = O(\tau^2)$ for $\theta = 1/2$ and $\psi^\tau = O(\tau)$ for the method with another weight parameter θ . This approach involves implementing a preliminary predictor stage for computing an approximate value of u^{n+1} by the simple explicit formula

$$B(\bar{u}^{n+1} - u^n) = \tau_n(f^n - Au^n) \equiv \tau_n r^n,$$

where B is a diagonal or another easily invertible matrix, and $\bar{u}^{n+1}$ is considered to be a predicted value of u^{n+1} . It can be interpreted as a zero iteration, $u^{n+1,0} = \bar{u}^{n+1}$, and corrected by m iterations of the form

$$\begin{aligned} B(u^{n+1,s} - u^n) &= \tau_n[\theta(f^{n+1} - Au^{n+1,s-1}) + (1 - \theta)(f^n - Au^n)], \\ s &= 1, \dots, m. \end{aligned}$$

This approach is called PC^m and in practice in a few iterations provides an acceptable small residual

$$r^{n+1,s} = \tau_n[\theta(f^{n+1} - Au^{n+1,s-1}) + (1 - \theta)r^n] - B(u^{n+1,s} - u^n)$$

An improved idea to choose the initial guess based on the least-squares method can be proposed (LSM, see [11]). Let us save several previous time-step solutions $u^{n-1}, \dots, u^{n-q}$, and compute the value $u^{n+1,0}$ by means of the linear combination

$$\begin{aligned} u^{n+1,0} &= u^n + c_1 v_1 + \dots + c_q v_q = u^n + Vc, \\ v_l &= u^n - u^{n-l}, l = 1, \dots, q, \\ c &= (c_1, \dots, c_q)^T \in R^q, \quad V = (v_1, \dots, v_q) \in R^{N,q}. \end{aligned} \quad (14)$$

Thus it follows from relation (14) that the initial residual $r^{n+1,0} = g^{n+1} - Cu^{n+1,0}$ of system (13) satisfies the equality

$$r^{n+1,0} = r^n - CVc.$$

Formally, here we can set $r^{n+1,0} = 0$ and obtain overdetermined SLAEs for the vector c :

$$Wc \equiv CVc = r^n, \quad W \in R^{N,q}.$$

The generalized normal (with a minimum norm and residual) solution of this system can be computed by the SVD (Singular Value Decomposition) algorithm or by the least squares method (LSM), which gives the same result in the exact arithmetic. The LSM gives the "small" symmetric system

$$Gc \equiv W^T Wc = W^T r^n, \quad G = V^T C^T C V \in R^{q,q}, \quad (15)$$

which is non-singular if W is a full-rank matrix. It is easy to verify that (15) implies the orthogonality property of the residual:

$$W^T r^{n+1,0} = 0. \quad (16)$$

Note that instead of the LSM approach (15), (16), it is possible to apply the so-called deflation principle [8], which uses the following orthogonality property:

$$V^T r^{n+1,0} = 0.$$

In this case to determine the vector c , we have to solve the SLAEs

$$Hc \equiv V^T C Vc = V^T r^n, \quad H \in R^{q,q}, \quad (17)$$

If this vector is computed from system (15) or (17), then the initial guess $u^{n+1,0}$ for SLAEs (13) is determined from (14). For solving a symmetric positive definite SLAEs

$$Cu^{n+1} = g^{n+1} \quad (18)$$

at each time step, we use the conjugate residual method in the Krylov subspaces based on an incomplete factorization algorithm in the Eisenstat modification as a preconditioner. For the matrix $C = D - L - U$, we define the explicit symmetric positive definite preconditioning matrix as

$$P = (M - L)M^{-1}(M - U), \quad M = \frac{1}{\omega}D - \theta S, \quad Se = \left(\frac{1-\omega}{\omega}D + LM^{-1}U\right)e, \quad (19)$$

where ω and θ are relaxation and compensation parameter, respectively, $e = \{1\}$ is the vector with unit entries, S and M are the diagonal matrices.

System (18) is transformed to the equivalent preconditioned system

$$\begin{aligned} \tilde{C}\tilde{u}^{n+1} &= \tilde{g}^{n+1}, \\ \tilde{C} &= M^{\frac{1}{2}}(D - L)^{-1}C(D - U)^{-1}M^{\frac{1}{2}} = \\ &= (I - \tilde{L})^{-1} + (I - \tilde{U})^{-1} - (I - \tilde{L})^{-1}(2I - \tilde{D})(I - \tilde{U})^{-1}, \\ \tilde{L} &= M^{-\frac{1}{2}}LM^{-\frac{1}{2}}, \quad \tilde{U} = M^{-\frac{1}{2}}UM^{-\frac{1}{2}}, \quad \tilde{D} = M^{-\frac{1}{2}}DM^{-\frac{1}{2}}, \\ \tilde{u}^{n+1} &= (I - \tilde{U})M^{\frac{1}{2}}u^{n+1}, \quad \tilde{g}^{n+1} = (I - \tilde{L})^{-1}M^{-\frac{1}{2}}g^{n+1}. \end{aligned} \quad (20)$$

To solve the obtained preconditioned SLAEs (20) with a symmetric positive definite matrix $\tilde{C}$, one can apply the conjugate residuals method

$$\begin{aligned} \tilde{r}^0 &= \tilde{g}^{n+1} - \tilde{C}\tilde{u}^{n+1,0}, \quad p^0 = \tilde{r}^0, \\ \tilde{u}^{n+1,i+1} &= \tilde{u}^{n+1,i} + \alpha_i p^i, \quad \tilde{r}^{i+1} = \tilde{r}^i - \alpha_i \tilde{C}p^i, \quad \alpha_i = \frac{(\tilde{r}^i, \tilde{C}\tilde{r}^i)}{(\tilde{C}p^i, \tilde{C}p^i)}, \\ p^{i+1} &= \tilde{r}^{i+1} + \beta_i p^i, \quad \beta_i = \frac{(\tilde{r}^{i+1}, \tilde{C}\tilde{r}^{i+1})}{(\tilde{r}^i, \tilde{C}\tilde{r}^i)}, \quad i = 0, 1, 2, \dots \end{aligned} \quad (21)$$

The stopping criterion of such iterations is as follows

$$\|r^{n+1,m}\| = \|\tilde{g}^{n+1} - Cu^{n+1,m}\| \leq \epsilon \|g^{n+1}\| \quad (22)$$

for some given tolerance $\epsilon \ll 1$. If condition (22) is satisfied, we set $u^{n+1} = u^{n+1,m}$ and go to the next time step.

5. Computational Experiments

We consider the following model problem: the computational domain of $\Omega = 120 * 120 * 60$ meters contains 1 or 4 wells parallel to the axis z and diameter 0.2 meters with length to equal 60 meters during 5-years. The medium coefficients take from [3] are equal to:

$$\begin{aligned} \rho^- c^- &= 1.62 * 10^6, & \rho^+ c^+ &= 2.04 * 10^6, \\ \lambda^- &= 1.332, & \lambda^+ &= 0.992. \end{aligned} \quad (23)$$

We consider the area with one shaft located at the center and four shafts located in a square, with a distance between the shafts of 1 m and the center of the square lying at the center of the area. The developed software packages have been tested on several problems with the analytical solution on a mesh of up to 2 000 000 nodes and more than 30 000 000 nonzero entries in a sparse matrix. The number of iterations of iterative sparse solvers depends on the matrix size but is less than 50 even for a big problem. Below is Figure 5 showing the spread of the thawing zone after 5 years.

When specifying the following physical parameters of the media and the Dirichlet 'weather' boundary conditions as presented in [4], we have got a qualitative picture of the spread of the freezing zone (see Figure 5) that coincides with that obtained in this paper. A direct comparison of quantitative values is impossible, since we calculated a well that does not have an additional heat-shielding layer, as in [4]. Nevertheless, we got a good coincidence of the qualitative picture and comparable sizes and shape of the freezing area (taking into account an additional thermal protection). Also, the results for a bunch of four wells arranged in a square with a side between the centers of 1 meter (see Figure 5) were obtained.

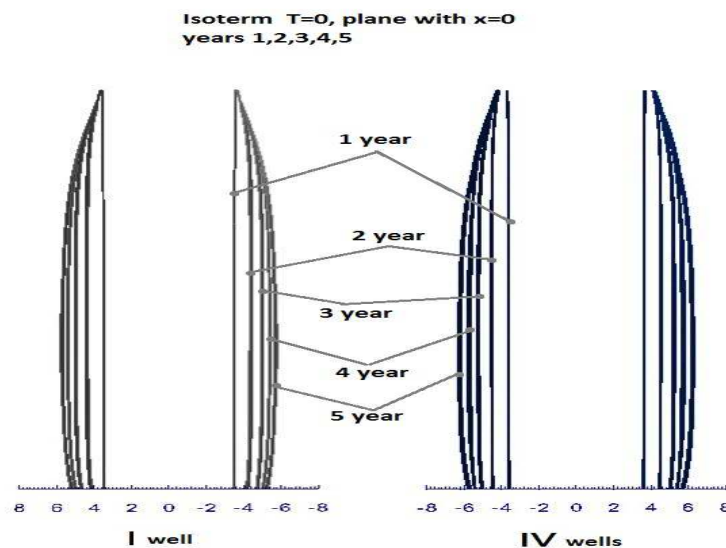


Figure 5. The temperature contours at $T = 0$ with an annual interval of 5 years with 1 year time step, in the case of the 1 and 4 wells.

The results obtained correspond to the physical sense, in comparison with the single-well option, and allow us to conclude that the technique proposed allows us to efficiently and with a sufficient accuracy simulate thermal fields. Also, other algorithms have produced the same results [14].

6. Conclusion

The results presented of computational experiments in 3D complex geometry domains with contrast material properties demonstrate the possibility of using the developed parallel software package to solve the problem of calculating the thermal field taking into account the phase transition. Using the adapted non-structured grids, choosing the initial guess in the iterative solver for SLAEs and a special parallel algorithm to efficiently using many-threads devices such as Intel Xeon Phi. In the future, it is planned to continue accelerating software through the use of algorithms with a fewer number of operations and memory accesses and increasing the parallelization efficiency.

Acknowledgments

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