Parallel Algorithm for Calculating the Dynamics of Tungsten Vapor Distribution

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Abstract. We consider an extended dynamic model of tungsten vapor distribution when the surface of a tungsten sample is heated by an electronic beam pulse. The parameters of the model are taken from the experiments on the Beam of Electrons for materials Test Applications (BETA) stand. This stand was designed in the INP SB RAS. The temperature in the sample is calculated from the two-phase Stefan problem. The temperature on the surface of the sample is taken as a boundary condition for the system of gas dynamics equations. A case of axial symmetry is considered. A parallel version of the algorithm, implemented using OpenMP technology, is presented.

1. Introduction
On the experimental stand BETA, the results of heating the tungsten plate by an action of a high-speed electron beam were obtained in [1]. Electrons with an energy of 80–90 keV heat the material in a layer thin as compared with the characteristic depth of heating of the material. The heat absorbed by the surface propagates into the material. A sample has dimensions of 25 mm × 25 mm and typical thickness of 4 mm. Since in such a short time the sample is heated to a depth of several hundred microns, the simulation region was a transverse section of the sample, a region of 12 mm × 3 mm. As for the time, the numerical simulation continued until the moment at which the last measurement of the surface temperature was made. To determine the acceleration of rotation of the melt, we need to determine the current distribution. To do this, the temperature of the sample and the vaporized gas must be calculated.

2. The Statement of the Problem
2.1. Stefan Problem
To determine the temperature on the heated surface, the temperature distribution in the sample is calculated based on the solution of the Stefan problem [2]. The position and speed of the
phase boundary depends on nonlinear coefficients. The condition at the free melt-solid boundary consists in the continuity of temperature and discontinuity of the heat flow due to the absorption or release of a known amount of heat. The novelty and complexity of the Stefan problem is mainly due to the necessity of a formulation of nonlinear boundary conditions describing the heating and evaporation of the material on its surface.

Stefan problem is used to calculate the temperature in the tungsten plate surface:

\[
\begin{cases}
    c(T)\rho^*(T) \frac{dT}{dt} = \frac{1}{r} \frac{\partial}{\partial r} \left( r \lambda(T) \frac{\partial T}{\partial r} \right) + \frac{\partial}{\partial z} \lambda(T) \frac{\partial T}{\partial z}, \\
    \left[ \lambda(T) \frac{\partial T}{\partial r} \right]_s = L_m v_n, \\
    (n, \nabla T) = W(t,r) - \frac{N(t,r)}{\gamma(T)}, \\
    W(t,r) = W_{\text{max}}(t) \cdot \exp(-A \cdot r^2),
\end{cases}
\]

where \( T(r,z,t) \) is the temperature, \( c(t) \) is the specific heat, \( \rho^*(T) \) is the density, \( \lambda(T) \) is the thermal conductivity, \( W(t,r) \) is the power of the heat flux on the surface \( \gamma \), \( N(t,r) \) is the power loss, \( n \) is the normal to the surface, and \( T_0 \) is the initial temperature, \( S \) is the free boundary, \( L_m \) is the enthalpy of the phase transition, \( v_n \) is the speed of the phase transition boundary. The melting point is \( T_m = 3695^\circ \text{K} \). At each time step in the numerical simulation, the variable \( W_{\text{max}}(t) \) is taken from the experimental data file, individual for each experiment. The power density \( W(r) \) has a radius distribution close to normal.

2.2. Gas Dynamic

At a temperature above 3000° K, significant metal evaporation begins. The plate is located in a vacuum. The temperature on the surface of the heated area in the center of the plate is significantly higher than at its edges. As it is shown in [2], the loss of energy for evaporation in a vacuum. The temperature on the surface of the heated area in the center of the plate is about 20% of the energy of pulsed heating. Numerical modeling is significantly higher than at its edges. As it is shown in [2], the loss of energy for evaporation in a vacuum. The temperature on the surface of the heated area in the center of the plate is about 20% of the energy of pulsed heating. Numerical modeling is necessary to determine the velocity and density distribution of the outgoing flow of vaporized tungsten. The mathematical model of gas flow from the sample surface is based on the solution of the system of gas dynamics equations:

\[
\begin{align*}
    \frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{v}) &= 0, \\
    \frac{\partial (\rho \vec{v})}{\partial t} + \text{div}(\rho \vec{v} \vec{v}) + P &= 0, \\
    \frac{\partial (\rho E)}{\partial t} + \text{div}(\rho E \vec{v}) &= 0, \\
    (\rho T) &= \frac{2}{3} \frac{M}{R} (\rho E - \frac{\rho \vec{v}^2}{2}), \quad \vec{v} = \frac{\rho \vec{v}}{\rho}, \quad T = \frac{(\rho T)}{\rho}, \quad P = \frac{R}{M} (\rho T),
\end{align*}
\]

where \( \rho \) is the gas density, \( \vec{v} = (v_r, v_z) \) is the gas velocity, \( P \) is the gas pressure, \( T(r,z,t) \) is the temperature, \( R \) is the gas constant, and \( M \) is the molar mass. The ratio for an ideal gas is chosen as the equation of state.

The Dirichlet conditions are set on the heated surface of the sample:

\[
\rho |_{\gamma} = \frac{1}{2} \left( \frac{R}{M} \right)^{-1} \frac{1}{T^*|_{\gamma}} \exp \left( a_1 - \frac{a_2}{T^*|_{\gamma}} \right), \quad v_z |_{\gamma} = \sqrt{\frac{5}{3}} \frac{R}{M} \sqrt{T^*|_{\gamma}},
\]

where \( T^*(r,t) \) is the temperature on the surface \( \gamma \) obtained from the calculation of Stefan problem (1). The symmetry boundary conditions are set on the axis and homogeneous Neumann boundary conditions are set on the other boundary parts. The surface temperature has an angle-symmetric distribution and increases non-linearly over time in accordance with the power of the heat flux \( W \).
3. Parallel Algorithm
To obtain the results, a parallel version of the program based on OpenMP technologies [3] has been developed. The program was implemented at the NKS-1P cluster (Computing Centre of SB RAS). To analyze the parallel algorithm, acceleration and efficiency are calculated using the formulas [4]:

\[
S_p = \frac{T_1}{T_p}, \quad E_p = \frac{\frac{T_1}{pT_p}}{\frac{S_p}{p}}
\]

Here \( T_n \) is the counting time for \( n \) cores, \( p \) is the number of cores. The acceleration is equal to the counting time on \( p \) cores compared to counting on one core.

3.1. Stefan Problem

![Graphs of the dependence of speedup (a) and efficiency (b) on the number of cores for the Stefan problem.](image)

Figure 1. Graphs of the dependence of speedup (a) and efficiency (b) on the number of cores for the Stefan problem.

The implicit implementation of the problem (1) by the tridiagonal matrix algorithm [5, 6] determines the standard parallel algorithm [7, 8]. The algorithm consists of the virtual distribution of data among the streams in OpenMP [3]. The forward step coefficients of the sweep are made private in each thread [4]. The dependences of acceleration and efficiency on the number of processors are shown in Figures 1 a and b.

3.2. Gas Dynamic
Instant heating up to 6-8 thousand Kelvin and an exponential increase in the gas density during evaporation on the surface leads to calculations with a very detailed time step. A complete calculation by the explicit Belotserkovsky method [9] requires 2 million time steps. The counting time decreases nonlinearly with an increase in the number of processors [10]. If on one core the calculation takes 5045 seconds, then on 64 cores it takes 192 seconds (Fig. 2). Accordingly, the acceleration increases (Fig. 3 a). For example, on 64 cores, computation is 26 times faster than with one core. The efficiency on two cores is 0.925, on 4 cores it is 0.92, on 8 it is 0.89 (Fig. 3 b). That is, up to 8 cores, the efficiency is very high. Then the efficiency starts to drop just as it is expected to be. On 64 cores, the efficiency is 0.41. This is due to the fact that an increasing of the number of cores, leads to increasing of synchronization delays. The calculation requires large amount of RAM, since space is required for 20 two-dimensional arrays of 10000 × 8000 64-bit memory cells.
3.3. Stefan Problem

![Stefan Problem graph](image)

**Figure 2.** Graphs of the dependence of time on the number of cores for the gas dynamic.

4. Conclusion

A parallel algorithm is presented for dynamic model of tungsten vapor distribution when the surface of a tungsten sample is heated by an electronic beam pulse. Instant heating up to 6-8 thousand Kelvin and an exponential increase in the gas density during evaporation on the surface leads to calculations with a very detailed time step. The algorithm consists of solving the Stefan problem by the tridiagonal matrix algorithm and solving a system of gas-dynamic equations by an explicit method. Using special operators of the OpenMP technology allowed us to get a good acceleration for the implicit method. The analysis of the parallel algorithm showed high acceleration and efficiency for this class of tasks.

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