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VILNIAUS GEDIMINO TECHNIKOS UNIVERSITETAS

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Introduction

Problem formulation

Topical problems of natural and technical investigations are rarely solved by applying analytical methods. These problems are described by systems of differential equations and are solved by applying numerical methods.

The methodology of problem solution includes the following mathematical modelling steps: description of formulated problems using mathematical models, selection of model parameters, development and analysis of numerical algorithms (analysis of approximation errors, solution stability, convergence and accuracy), implementation of algorithms, application of parallel algorithms, comparison of mathematical experiments with the results obtained in real experiments.

Topicality of the problem

In the dissertation mathematical modelling problems in the design of electrical cables and cable fibres in modern vehicles, and of the heating of metals or semiconductors by ultra short (pico- or femtosecond) laser pulses are investigated.

During the past decade the number and volume of electrical cables in vehicles, airplanes and other mobile equipments have increased significantly. The main task for engineers is to determine the optimal cross-section area of cables in order to reduce the total volume of cable installation. In loaded electrical wires current generates heat, therefore the temperature of the cable is an increasing function of the time. It is important to mark, that the temperature of the cable is bounded by maximal temperature.

Main stages in solving the electrical cable bundle optimization problem may be defined as follows:

- Creation of simplified (1D and 2D) mathematical models for calculation of heat transfer in cable bundles. These models should not be too complex, because it is important to develop models, that can be used when actual physical experiments are being changed by virtual (computer) modelling.
- 1D and 2D problem discretization, development and analysis of numerical algorithms.
- Model identification phase. Although characteristics of wire materials and air (air gaps between wires) are well known, one requires determining the so-called “mixed” conductivity coefficient of the wire isolation material and air by using the inverse problem solution method.
- Application of parallel algorithms. It is typical, that the direct problem of temperature distribution in electrical cables is solved by taking different sets

of parameters many times, therefore it is important to reduce the time of solving the direct problem by developing robust and efficient parallel numerical algorithms.

- Optimization stage. Geometric parameters of cable bundles shall be optimized by using the method of greedy search strategy in such a way, that the total volume of cable installation in a device would be reduced. Therefore, it is important to develop a parallel optimization algorithm. The cable bundle optimization problem belongs to the class of combinatorial (of non-polynomial complexity) problems, thus only heuristic algorithms, which are based on the methods of greedy strategies, are used.

In the dissertation material removal processes by ultra short (pico- or femtosecond) laser pulses are investigated. Since laser pulse is very short, the classical Fourier’s law is not valid. For metals the initial heating process is described using hyperbolic two temperature method, which includes the inertia of heat flow. This model provides a frame work for all models of laser ablation of metals and semiconductors.

For longer laser pulse hyperbolic two temperature model is simplified to the parabolic two temperature model, which may be simplified to the parabolic one temperature model. In most cases numerical methods, which would suit for both cases (hyperbolic and parabolic type of equations), are not effective.

The hyperbolic two temperature model allows an accurate modelling of the initial heat ablation (elimination) phase, when the metal is affected by ultrashort laser pulses. Therefore, it is worth to examine this model numerically and present an algorithm for its calculation in order to be able to simulate virtually other laser heating phases: the gas dynamics of laser ablation of materials, the process of metal ablation including plasma spread and absorption.

Research object

The main research objects of the dissertation are application and analysis of numerical methods of modelling heat processes in laser and electro-thermal technologies, also, the development and analysis of effective parallel algorithms used to make computational experiments.

Aims of the work

The aim of this dissertation is to create mathematical models and their numerical algorithms of heat exchange in cable bundles, which will enable the virtual simulation of temperature distribution in electrical cables and optimization of geometric parameters of cables.

The second aim is to create mathematical models and their numerical algorithms of laser effects on metals allowing the simulation of material heating and removal processes.

Tasks of the work

The main tasks of the work are the following:

1. to create the simplified (1D and 2D) mathematical models, which would describe heat exchange in composite materials, and to develop sequential and parallel algorithms of their numerical analysis;
2. to create the sequential and parallel optimization algorithms, that allow to determine the optimum area of cable cross-section, in order to solve problems of heat exchange in cable bundles.
3. to create the numerical algorithm for the analysis of the hyperbolic two temperature model, which would be applied to different lengths of a laser pulse (for solving both hyperbolic and parabolic equations) and would allow to determine other phases (the depth of heating, gas dynamics) of metal laser heating.

Methodology of research

The methodology used in this dissertation work consists of the numerical solution methods of partial derivative differential equations, their convergence and stability analysis, parallel algorithms, their complexity and scalability analysis, application of virtual experimental simulations.

Scientific novelty

There were created methods for realization of the full mathematical modelling cycle and corresponding sequential and parallel algorithms, which will enable the simulation of temperature distribution in electrical cables, optimization of their geometrical parameters, and modelling of processes of metal heating by laser and removal of the material.

Practical value

A part of the material, used in this work, was collected during the participation in the project E!3691 OPTCABLES "*Optimization of cable harness*" of the European research, development and cooperation program EUREKA, during the period of September 2006–December 2009. The research results were used in the Lithuanian high technology project, GRIDGLOBOPT "*Global Optimization of Complex Systems Using High Performance Computing and Grid Technologies*". Research results of ablation studies conducted during the period of preparation for the dissertation work were used in the Lithuanian high technology project, FEMTOAPDIRBIMAS “*Laser micromachining and prototyping with high repetition rate femtosecond pulses”*, during the period of April 2007–December 2009.

Defended propositions

1. Mathematical models of heat conduction in composite materials and the corresponding numerical sequential and parallel algorithms, which allow an effective calculation of temperature distribution in cable bundles, are developed;
2. Parallel optimization algorithm for reduction of geometrical parameters of cables based on the greedy search strategy is developed;
3. Numerical algorithm for the analysis of the hyperbolic two temperature model, which would be applied to calculate an initial ablation phase with different relaxation times, is developed.

The scope of the scientific work

The doctoral dissertation consists of the introduction, three chapters, conclusions, the list of references and the list of author’s publications. The scope of the dissertation: 105 pages, 16 figures, 10 tables. In the work 145 references are cited. The results of doctoral dissertation are published in 6 publications. The results were presented at seven national and five international conferences. The language of the doctoral dissertation is Lithuanian. The first chapter is dedicated to the overview of scientific literature and the introduction of the concepts of thermal processes in laser and electrothermal technologies, and solved equations. The second chapter presents mathematical models of heat conduction in electrical cables in cylindrical and rectangular areas, the corresponding numerical algorithms and the parallel algorithm of temperature distribution in cables. The optimization algorithm for reduction of geometrical cable parameters is developed and the parallel optimization algorithm is presented. The third chapter presents mathematical models of laser-heated metal, the numerical algorithm of the hyperbolic mathematical model and the gas dynamics model of the heated material.

1. The overview of numerical modelling of thermal processes in laser and electrothermal technologies

Optimization of many technological processes is a very important feature: the main aim is to reduce weight, volume, and energy consumption of a product or device with minimal infringements when processing a product.

During the past decade the number and volume of electrical cables in vehicles, airplanes and other mobile equipments have increased significantly.

The base of electrical installation in middle-class cars is a cable bundle, in which the number of cables normally does not exceed 42, but it is likely that by improving a design of device, comfort, specification and safety the volume of cables shall only increase in the future. However, these cables need to be placed in low-volume spaces. Therefore, the main task for engineers is to determine the optimal cross-section area of cables in order to reduce the total volume of cable installation. Usually the geometry of cable bundles is cylindrical in a vehicle, but in some cases the geometric shape can be tailored to a specific part of a vehicle. For example, cable bundles installed in the roof of a vehicle and in heated spots for coffee cups (in order to keep coffee warm for a longer time) has a flat shape.

When developing mathematical models and their numerical algorithms, it is important to take into account, that heat is spreading in a composite material and that the jump of coefficients of material diffusion can be very large. Solving linear equations with discontinuous coefficients is a tedious task. In this case, the discrete values of temperature in metal areas are susceptible to changes in temperature on the outside and iterations converge slowly.

The development of new technologies is tending not only to mobilize devices, but also to increase their operational efficiency. Laser ablation is a process of producing small units, sections and ridges by evaporation of a material. The use of femtosecond pulses enables an effective and qualitative processing of even those materials that possess characteristics of high heat conductivity and low melting temperature. In this way less heat is transmitted to a lattice than it would be transmitted when using nanosecond and picosecond laser pulses. Therefore, molten layer, micro cracks and shock waves do not occur and a product structure is not violated.

An interaction of laser radiation and material acquires a different nature, when exposed to extremely short pulses. The ultrashort laser pulse does not end until hydrodynamic transportation starts. This phase of material heating for metals and semiconductors is described with the two-temperature diffusion model (Kaganov *et al* 1957). However, it is worth to analyze the impact of heat inertia on the dynamics of material heating process when using picosecond and femtosecond laser pulses not only in metal materials. The modified Fourier's Law says that the inertia of heat flow is fundamentally changing the transfer of heat in a material. During initial stages of material heating with short pulses the same material acts as if it possesses a very low heat transfer coefficient. Thus, the material can be heated up to much higher temperature levels compared with the longer pulses of the same energy density. During this process heat waves, which move at a constant speed and reflect from the media walls, are formed in the material.

Therefore, it is necessary to use the modified two temperature model, which also includes the inertia of heat flow, when heating a metal with ultrashort (picosecond or femtosecond) laser pulses (Chen, Berau 2001; Huttner 2009). When relaxation times are equal to zero, the hyperbolic two temperature model is simplified to the parabolic two temperature model, which may be simplified to the one temperature model. This hyperbolic two temperature model can be used for the numeric analysis of heating thin metal films by ultrashort laser pulses.

Coefficients of the electron system and a lattice depend on temperature in this model. Two phases can be distinguished: firstly, electrons are heated due to the absorption of laser radiation, and then their energy is transmitted to the lattice. A term describing the energy transmission going from electrons to the lattice is also dependant on temperature.

Numerical methods for solving hyperbolic heat conduction problems were suggested in works of Glass *et al* (1985, 1987), Haitian, Qiang (2003), Kar *et al* (1992) and Sarra (2003). However, these studies are not sufficient for the development of the two temperature algorithm, because many hyperbolic problems are addressed here only in one temperature cases, thus oscillation of solutions occur and there is no stability and convergence analysis addressed. In most cases numeric algorithms, which would suit for both cases (hyperbolic and parabolic type of equations), are not effective (Manzaro et al 1999). The hyperbolic two temperature model provides a framework for all models of laser ablation of materials.

The hyperbolic two temperature model allows an accurate modelling of the initial heat ablation (elimination) phase, when the metal is affected by ultrashort laser pulses. Therefore, it is worth to examine this model numerically and to present an algorithm for its calculation in order to simulate virtually the other laser heating phases: the gas dynamics of laser ablation of materials, the process of metal and dielectric ablation including plasma expansion and absorption

2. Optimization of electrical cables

In today's vehicle production it is very important to be able to select right geometrical and physical parameters of electrical cables (insulated cable bundles), which transmit energy or information. The aim is to ensure a reliable and secure transfer of energy and information, using a minimum amount of metal (copper), because this allows reducing the cost of a device and space that is occupied in a vehicle. A design of cables with optimum diameters in a mobile device depends on the specification and design of that device. Different standards must be applied for the design of cables of mobile devices compared to fixed installations. Usually the geometry of cable bundles is cylindrical in a vehicle, but in some cases the geometric shape can be tailored to a specific part of a vehicle (e. g. cable bundles installed in the roof of a vehicle have a flat shape). In loaded electrical wires current generates heat, therefore the temperature of the cable is an increasing function of the time. It is important to mark, that the temperature of the cable is bounded by maximal temperature. Thus, the main aim of this problem is to determine the optimal conductor cross sections for continuous electrical loads in mobile systems.

This chapter presents the mathematical models and numerical algorithms for the heat transfer simulation in composite materials. The main features of the problem deal with discontinuous diffusion coefficients and nonlinear convection and radiation boundary conditions. The differential problems are approximated by the finite volume discrete schemes. Linearization of the nonlinear problems is done by using the predictor-corrector and Picard methods. The obtained systems of linear equations are solved by using BiCGSTAB iterative method with Gauss Seidel type preconditioner (in cylindrical cables) and FCG iterative method with AGMG preconditioner (in flat cables). We note that the solution of such systems is a challenging task, since the diffusion coefficient is a discontinuous function and the jump of the coefficient is large. In such situations the discrete value of the temperature in the metal region starts to be non-sensitive to outside changes of the temperature and iterations converge slowly. Efficient solvers of such problems can be obtained by using multigrid algorithms.

In this section we also investigate the stability and convergence of the 1D differential problem in composite material. A discrete problem is constructed using finite volume method, a special attention is given to the approximation of the nonlinear Robin boundary conditions. The Picard iterative method is used to linearize the nonlinear discrete problem, the convergence of iterations is also proved.

Mathematical model of heat conduction in the cylindrical conductor

For a given bundle of electrical cables we consider a domain, $D \times (0, t_F]$, where $D = \{X = (x_1, x_2) : x_1^2 + x_2^2 \le R^2\}$, R is the radius of outer isolation of the bundle. All wires which make up the cable bundle need to fulfil electrical and thermal requirements. Thus, temperature of the wire isolation must not exceed a maximal permissible value. The temperature rise is essentially caused by ohmic heating of current-carrying parts. The main mechanisms of heat transfer are: conduction in solid bodies (conductors, PVC isolation); conduction in the air and PVC mixture (the heat conductivity coefficient of the mixture should be identified by using the inverse problem solution method); convection and radiation from the outer side of the bundle isolation to the environment.

Let $T(X, t)$ describe a distribution of the temperature in electrical cables. The mathematical model consists of the parabolic differential equations:

$$c(X,T)\rho(X)\frac{\partial T}{\partial t} = \sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left(k(X)\frac{\partial T}{\partial x_i}\right) + f(X,T);\ \ (X,t) \in D \times (0,t_F] \tag{1}$$

subject to the initial and boundary conditions: $T(X,0) = T_a,\ X \in \overline{D} = D \cup \partial D$

$$k(X,T)\frac{\partial T}{\partial \eta} + \alpha_k(T)\big(T(X,T) - T_a\big) + \varepsilon\sigma\left(\tilde{T}^4 - \tilde{T}_a^4\right) = 0,\ \ X \in \partial D\ \cdot$$

The continuity conditions: $[T(x,t)] = 0,\ \ [k\,\partial T/\partial x_i] = 0$ are specified at the points of discontinuity of coefficients. In the model $c(X, t)$ is the specific heat capacity, $\rho(X)$ is the density, $k(X)$ is the heat conductivity coefficient, $f(X, T)$ is the density of energy source, T_a is the temperature of the environment, $\tilde{T}$ is the temperature in the Kelvin scale, I is a direct electrical current.

Mathematical model of heat conduction in the flat conductor. In domain $D = (0, L_1) \times (0, L_2)$ we solve the nonlinear stationary problem, which describes a distribution of the temperature $T(X)$ in domain D. This domain defines a composite structure of metal and isolation materials. The mathematical model consists of the elliptic differential equation:

$$-\sum_{i=1}^{2}\frac{\partial}{\partial x_i}\left(k(X)\frac{\partial T}{\partial x_i}\right) = \left(\frac{I(x)}{A}\right)^2 \rho_0(1 + \alpha_\rho(T - 20)),\ \ X \in D,$$

subject to the symmetry condition on $\partial D_1 = \{(0, x_2), x_2 \in [0, L_2]\}$

$k(X)\dfrac{\partial T}{\partial x_1} = 0, X \in \partial D_1$ and the nonlinear boundary conditions on the remaining part of the boundary:

$$k(X)\frac{\partial T}{\partial \eta} + \alpha_k(T)\big(T(X) - T_a\big) + \varepsilon\sigma\left(\tilde{T}^4 - \tilde{T}_a^4\right) = 0,\ \ X \in \partial D \setminus \partial D_1$$

The standard continuity conditions specified at the points of the discontinuity of coefficients: $[T(X)] = 0,\ \ [k\,\partial T/\partial x_i] = 0$. We note, that the thickness of metal, compared to thickness of the isolation material, is very thin.

Optimization algorithm. Let $G = \{d_k, k = 1,...K\}$ be a set of feasible diameters of wires and $D = \{d_{k_1},...,d_{k_M}\}, d_{k_M} \in G,\ m = 1,...,M -$ a set of diameters in a bundle from M cables. The critical scenarios of loads of electrical cables are defined by: $S_j = \{I_m^j, m = 1...M\}, j = 1,...J$, where

I_j^m defines the current applied to the *m*-th wire in the *j*-th scenario. These scenarios are selected from a set of regimes which are important for the design of a specific car. The objective function *W* defines the total mass of metal in all wires. It is defined by the following formula: $W(d_{k_1},...,d_{k_M}) = \frac{\rho\pi}{4}\sum_{m=1}^{M} d_{k_m}^2$, where ρ is the density of the metal. Our main aim is to solve the following optimization problem:

$$\min_{d_{k_m}\in, T\le T_{\max}} W(d_{k_1},...,d_{k_M}) = W(d^0{}_{k_1},...,d^0{}_{k_M}) . \qquad (2)$$

Here $T_{\max}$ is the critical (e.g. melting) temperature, *T* is the maximal temperature of electrical wires with respect to all load scenarios $T = \max_{1\le j\le J}\max_{1\le m\le M} U_m(S_j)$, and $U_m(S_j)$ denotes the simulated temperature of the *m*-th wire when S_j load scenario is used.

In general, optimization problem (2) belongs to the class of combinatorial search problems. In order to find an approximate solution we propose the following heuristic, which is based on a greedy search algorithm (see, Fig.1).

```
OptimalSetOfWires
Begin
(1)  $D$ = SelectInitialSetOfWires( );
(2)  while ( $T \le T_{\max}$) do
(3)        SaveOptimalSetOfWires($D$);
(4)        $oK$ = FindLighterSetOfWires($D,G$);
(5)        if (oK = = 1) do
(6)          for (j = 0; j< J; j++) do
(7)            $\Omega_j$ = GenerateSetOfDistributions($S_j$, $D$);
(8)            $T_j$ = ComputeTemperature ($\Omega_j$);
             end for do
(9)          $T = \max_{0\le j\le J} T_j$;
        else
(10)         $T$ = 2 $T_{\max}$
        end if do
    end while do
end OptimalSetOfWires
```

Fig. 1. Optimization algorithm

Parallel optimization algorithm. The proposed above optimization algorithm has at least three parallelization levels:

- First, in step (6) all subproblems for different load scenarios are independent and can be solved in a parallel way.
- The second parallelization level is obtained considering the solution of each of *J* subproblems.
- At the final parallelization level, the temperature inside of a bundle of electrical cables can be simulated by using the parallel version of the discrete algorithm.

Here we consider two parallel versions of the given optimization algorithm. The first one uses a very popular general approach to construct parallel algorithms: the master-slave paradigm. It is applied in heterogeneous environments of varying computational complexity of subproblems and/or non-uniform and non-dedicated parallel architecture. This approach introduces very naturally the dynamical load-balancing techniques. The second parallel version of the optimization algorithm is based on data distribution paradigm.

3. Numerical simulation of metal ablation using ultrashort laser pulses

Over the last few years, ablation processes, affected by ultrashort laser pulse, have been widely investigated (Bulgakova, Bulgakov 2002; Chen, Beraun 2001; Phipps 2007). The use of femtosecond laser pulses opened attractive possibilities for the high quality microprocessing of many materials, simultaneously minimizing their violations. Laser ablation (laser plasma evaporation) usually happens due to the thermal effects, which appear when a laser beam interacts with the surface of processed materials.

The following steps will be made in the modelling of the material removal processes:

- During the initial stage we will estimate temperature diffusion in the metal lattice, when short (duration of ~100 fs) pulses are present. The hyperbolic two temperature model will be used for simulations.
- During the second stage we will estimate the depth of ablation crater using a specific ablation mechanism. Such criteria will allow us to determine initial conditions for formation of a highly heated gas plume.
- During the third stage, when plume expands, we will solve equations of gas propagation dynamics, including the Van der Waals equation, and determine an interaction among material atoms (in an imperfect gas case).

Hyperbolic two temperature model. When the ultrashort laser pulse interacts with the surface, here two stages can be pointed out. Firstly, electrons are heated due to the absorption of laser radiation, secondly, their energy is transferred to the lattice. For metals and semiconductors these processes are usually described using the two-temperature diffusion model (Kaganov et al 1957). However, for very short laser pulses it is worth to investigate thermal inertia effect on the dynamics of thermal energy transfer (Chen, Beraun 2001; Huttner 2009). According to the improved Fourier's law thermal energy transfer in the material is changed by the lag of thermal flux. In the primary stages of material heating with short impulses, the material itself reacts as if it had a very low coefficient of heat transfer. Thus, the material can be heated up to much higher temperatures in comparison with the impulses of the same energy density, but of longer period. For the metals this heating process is described using hyperbolic two-temperature model:

$$
\begin{aligned}
&C_E(T_E,T_L)\frac{\partial T_E}{\partial t} = -\frac{\partial q_E}{\partial z} - \Gamma(T_E,T_L) + \alpha_a(1-R)If(t)e^{-\alpha_b z},\\
&\tau_E\frac{\partial q_E}{\partial t} + q_E = -k_E(T_E,T_L)\frac{\partial T_E}{\partial z},\\
&C_L(T_E,T_L)\frac{\partial T_L}{\partial t} = -\frac{\partial q_L}{\partial z} + \Gamma(T_E,T_L),\\
&\tau_L\frac{\partial q_L}{\partial t} + q_L = -k_L(T_E,T_L)\frac{\partial T_L}{\partial z},
\end{aligned}
\qquad (1)
$$

where T_E and T_L are temperatures of electrons and the lattice, respectively, C_E, C_L are heat capacities per unit volumes, k_E, k_L are thermal conductivities, $\Gamma(T_E,T_L)$ denotes the electron-lattice coupling factor. In the laser heat source R is reflectivity, α_a is a light absorption coefficient, α_b denotes electrons ballistic effect. I is the maximum of pulse intensity and $f(t)$ defines the pulse shape. The initial conditions describe a stationary state of the system: $T_{E,L} = T_*$, $q_{E,L} = 0$, where T_* is the ambient temperature. Boundary conditions on the substrate surface are given by:

$$
\begin{aligned}
&-k_{E,L}\frac{\partial T_{E,L}(0,t)}{\partial z} + h_{E,L}(T_{E,L}(0,t) - T_*) = 0,\\
&k_{E,L}\frac{\partial T_{E,L}(Z,t)}{\partial z} + h_{E,L}(T_{E,L}(Z,t) - T_*) = 0.
\end{aligned}
$$

The parameters of materials, heated to very high temperatures, depend on the temperature. The term, describing the transfer of energy from the electron system to the lattice, also depends on the temperature. Thus, the numerical analysis of hyperbolic two-temperature model is rather complex and requires a deep theoretical investigation.

Numerical methods are introduced for the two-temperature hyperbolic heat conduction problem. We investigate the explicit and fully implicit Euler type scheme for the time integration of the nonstationary problem. Space derivatives are approximated by finite difference scheme of the second order of accuracy.

The boundary conditions are also approximated in a consistent way. The stability analysis is done in the L_2 and energy norms for a simplified one-temperature equation and the system of two equations describing the mass balance of temperature and the flux. This analysis gives us a priori information on the properties of the introduced approximations and forms a basis for the stability and convergence analysis of the full nonlinear two-temperature hyperbolic heat conduction model.

In this section we have formulated mathematical models describing the interaction of ultrashort laser pulse with metals. For the numerical analysis of the two-temperature model a homogeneous linear one-temperature hyperbolic model is considered. A family of finite difference schemes is constructed and the approximation and stability is investigated for the two most interesting schemes. By using the spectral and energy methods the sufficient stability conditions are obtained. A finite difference scheme for one temperature system of equations is constructed on a staggered space grid. In this section we investigate the convergence and the complexity of the numerical algorithm. We propose numerical methods for systems of nonlinear hyperbolic equations and present the results of numerical experiments.

General conclusions

Methods and tools of virtual experimental simulation are created here to solve problems of the optimization of real technological processes (reduction of a device weight, processing of materials with minimal violations), which are examined in this dissertation work.

1. The following stages of mathematical modelling are proposed to optimize electrical cable bundles:

    - Several complete and simplified one-dimension and two-dimension mathematical models of composite materials were proposed to solve the problem of heat exchange in cable bundles. These models allow to determine main processes, presented in the analyzed materials, and to calculate temperature diffusion in cylindrical and rectangular conductors;
    - Stable sequential and parallel algorithms were formulated and investigated for the developed mathematical models and methods for the identification of unknown model parameters were suggested in this work. Results of computational experiments were compared with the experimental data and they showed, that the models are adequate and suitable for the optimization of geometrical parameters of cable bundles;
    - In order to optimize cable parameters the direct problem should be solved many times, thus the parallel optimization algorithm was developed (two strategies for solving this algorithm were realized: master-slaves and data

distribution paradigms). Combinatorial search optimization algorithm, which is based on greedy search strategy, allows effective reduction of the mass of cable bundles.

- The optimization algorithm can be applied to various architectures of parallel computers and to realize other multi-level algorithms.

2. There were obtained the following results related to numerical simulation of metal ablation:

- Since the processes of heat transfer and hydrodynamic ablation take place on different time scales when affected with an ultrashort laser pulse, mathematical models and algorithms of numerical analysis of these processes (metal heating, melting and evaporation) were created and investigated. These algorithms enable a simple definition of the ablation depth of pulse duration and energy density.
- The Fourier's Law of conduction does not consider a thermal relaxation phase, which becomes important when the process time becomes short. Numerical methods ant their algorithms (the stability of which does not depends on a relaxation parameter) of hyperbolic two temperature model (which estimates the time of thermal relaxation) allow to simulate the distribution of the temperature (the initial ablation phase), when different values of relaxation parameters are chosen.

List of published works on the topic of the dissertation

In the reviewed scientific journals

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Čiegis, R.; Jankevičiūtė, G. 2009. Parallel numerical solver for the simulation of the heat conduction in electrical cables. In: Čiegis, R.; Henty, D.; Kagstrom, B.; Žilinskas, J. EDS, *Parallel Linear Algebra and Optimization: Advances and Applications*. Springer Optimization and Its Applications. Springer. 27: 211–216, ISSN 1931-6828, ISBN 978-0-387-09706-0 [Conference Proceedings Citation Index (Web of Science)].

Čiegis, R.; Jankevičiūtė, G.; Dementjev, A. 2007. Dviejų temperatūrų hiperbolinio tipo šilumos pernešimo modelis ir jo analizė. X Lietuvos jaunųjų mokslininkų konferencijos *Lietuva be mokslo – Lietuva be ateities* medžiaga: Matematika ir informatika. p. 193–203, ISBN 978-9955-28-144-3.

About the author

Gerda Jankevičiūtė was born in Utena on 10 of May 1979.

Bachelor of Science in Applied Mathematics, Faculty of Fundamental Science, Kaunas University of Technology, 2001. Master of Science in Applied Mathematics, Faculty of Fundamental Science, Kaunas University of Technology, 2003. PhD Student in Mathematics, Vilnius Gediminas Technical University and lecturer at Mathematical Modelling department in Vilnius Gediminas Technical University, September 2006 to present.

ŠILUMINIŲ PROCESŲ LAZERINĖSE IR ELEKTROTERMINĖSE TECHNOLOGIJOSE MATEMATINIS MODELIAVIMAS

Problemos formulavimas. Aktualūs gamtos ir technikos tyrimo uždaviniai yra retai sprendžiami analiziniais metodais. Nagrinėjami uždaviniai yra aprašomi diferencialinėmis lygtimis ir dažniausiai sprendžiami skaitiniais metodais.

Sprendžiamų uždavinių metodiką apima šie matematinio modeliavimo etapai: suformuluotų uždavinių aprašymas matematiniais modeliais, modelių parametrų parinkimas, skaitinių algoritmų sudarymas ir tyrimas (aproksimacijos paklaidų, sprendinio stabilumo, konvergavimo ir tikslumo analizė), algoritmų sudarymas, lygiagrečiųjų algoritmų taikymas, skaičiavimo eksperimentų rezultatų palyginimas su realaus eksperimento rezultatais.

Darbo aktualumas. Disertacijoje nagrinėjama elektros kabelių ir kabelių pluoštų projektavimo šiuolaikiniuose automobiliuose, metalų arba puslaidininkių kaitinimo ultratrumpais (piko- arba femtosekundiniais) lazerio impulsais matematinio modeliavimo uždaviniai.

Vystantis naujoms technologijoms elektros kabelių skaičius ir ilgis automobiliuose didėja, todėl inžinieriams pagrindinis tikslas yra, kaip nustatyti optimalų laido skerspjūvio plotą, kad būtų sumažinta bendra laidų masė įrenginyje. Elektros srovė, tekėdama laidu, generuoja šilumą, dėl ko kyla jo temperatūra. Kuo didesnis srovės tankis, tuo didesnė temperatūra yra pasiekiama stacionariame režime. Siekiama, kad ši temperatūra neviršytų izoliacijos lydymosi temperatūros.

Laidų pluoštų optimizavimo elektros kabeliuose uždavinio etapai gali būti išskaidyti taip:

- Supaprastintų (1D ir 2D) matematinių modelių šilumos mainams laidų pluoštuose apskaičiuoti sudarymas. Modeliai neturi būti per daug sudėtingi, svarbu sukurti modelius, kurie gali būti naudojami keičiant realius fizinius eksperimentus virtualiuoju (kompiuteriniu) modeliavimu.
- 1D ir 2D uždavinių diskretizacijos etapas. Diskrečiųjų tinklų ir skirtuminių schemų sudarymas, netiesinių schemų linearizavimas ir diskrečiųjų uždavinių realizavimas. Diskrečiųjų uždavinių stabilumo ir konvergavimo analizės tyrimas.
- Modelių identifikavimo etapas. Nors laidų medžiagų ir oro (oro tarpai tarp laidų) savybės gerai žinomos, tačiau pasirinktame modelyje atvirkštinio uždavinio metodu yra būtina rasti mišinio (iš laidų izoliacijos medžiagos polivinilchlorido ir oro) šilumos laidumo koeficientą.
- Lygiagrečiųjų algoritmų taikymas. Sprendžiant laidų pluošto optimizavimo uždavinį naudojami variantų perrinkimo metodai, kai uždavinį tenka spręsti daug kartų imant vis kitus parametrų rinkinius, todėl svarbu sumažinti tiesioginio uždavinio sprendimo laiką naudojant efektyvius lygiagrečiuosius algoritmus.
- Optimizavimo etapas. Sukūrus matematinius modelius ir šiuos modelius identifikavus pereinama prie mobiliųjų įrenginių laidų pluoštų geometrinių parametrų optimizavimo. Laidų pluoštų geometriniai parametrai godžiosios strategijos algoritmu turi būti optimizuoti taip, kad būtų sumažinta bendra laidų masė įrenginyje. Todėl svarbu sukurti lygiagretų optimizavimo algoritmą. Laidų pluoštų optimizavimo uždavinys priklauso kombinatorinių (nepolinominio sudėtingumo) uždavinių klasei, todėl pakankamai didelės apimties skaičiavimams apsiribojama euristiniais algoritmais, kurie remiasi godžiosios strategijos ir variantų perrinkimo metodais.

Darbe taip pat nagrinėjami metalų pašalinimo procesai, kai juos veikia ultratrumpieji (pikosekundiniai ir femtosekundiniai) lazerio impulsai. Abliacijos lazerio impulsais metu vyksta daug skirtingų fizikinių procesų. Kadangi lazerio impulsas yra labai trumpas, klasikinis Furjė dėsnis negalioja. Metalams ir puslaidininkiams pradinis medžiagos kaitinimo etapas yra aprašomas dviejų temperatūrų hiperboliniu modeliu, kuriame įvertinamas šiluminio srauto inertiškumas įvedant relaksacijų trukmes. Šis modelis sudaro pagrindą visuose lazerinės abliacijos modeliuose. Ilginant lazerio impulso trukmę, hiperbolinis modelis virsta paraboliniu dviejų temperatūrų modeliu, kuris gali būti supaprastintas iki parabolinio vienos temperatūros modelio. Daugeliu atveju skaitiniai algoritmai, kurie tiktų abiems atvejams (hiperbolinių ir parabolinių tipų lygtims) nėra efektyvūs. Dviejų temperatūrų hiperbolinis modelis leidžia pakankamai tiksliai modeliuoti pradinę šiluminę abliacijos (pašalinimo) fazę, kai metalą veikia ultratrumpasis lazerio impulsas, todėl aktualu šį modelį ištirti skaitiškai ir pateikti jo skaičiavimo algoritmą, kad virtualiojo eksperimento būdu galima būtu modeliuoti kitas lazerio kaitinimo fazes – lazerinės medžiagų abliacijos dujų dinamiką, metalų abliacijos procesą, įskaitant plazmos plėtimąsi ir sugertį.

Tyrimų objektas. Skaitinių metodų, skirtų šiluminių procesų lazerinėse ir elektroterminėse technologijose modeliavimui, pritaikymas ir jų analizė. Efektyvių lygiagrečiųjų algoritmų, naudojamų skaitiniams eksperimentams atlikti, sukūrimas ir analizė.

Darbo tikslai. Sukurti šilumos mainų kabelių pluoštuose matematinius modelius ir skaitinės analizės algoritmus, kurie virtualiojo eksperimento būdu leistų modeliuoti temperatūros pasiskirstymą elektros kabeliuose ir optimizuoti geometrinius laidų parametrus. Sukurti lazerio poveikio metalui matematinius modelius ir jų skaitinės analizės algoritmus, leidžiančius modeliuoti medžiagos kaitinimo ir pašalinimo procesus.

Darbo uždaviniai

1. Sudaryti supaprastintus matematinius modelius, kurie aprašytų šilumos mainus kompozicinėse medžiagose (metalo ir izoliacijos). Sukurti jų skaitinės analizės nuosekliuosius ir lygiagrečiuosius algoritmus.
2. Šilumos mainų uždaviniui elektros kabelių pluoštuose spręsti sukurti nuoseklų ir lygiagretų optimizavimo algoritmą, leidžiantį nustatyti optimalų laido skerspjūvio plotą.
3. Sukurti skaitinės analizės nuoseklųjį skaičiavimo algoritmą dviejų temperatūrų hiperboliniam modeliui, kuris būtų taikytinas įvairiems lazerio impulso ilgiams (tiek hiperbolinėms, tiek parabolinėms lygtims spręsti) ir leistų apskaičiuoti metalo kaitinimo lazeriu kitas fazes (išdeginimo gylį, dujų dinamiką).

Tyrimų metodika. Dalinių išvestinių diferencialinių lygčių skaitiniai sprendimo metodai, jų konvergavimo ir stabilumo analizė, lygiagretieji algoritmai, jų sudėtingumo ir išplečiamumo analizė, vitualaus eksperimentinio modeliavimo tyrimo metodai

Darbo mokslinis naujumas ir jo reikšmė. Sukurti matematinio modeliavimo ciklą realizuojantys metodai ir jų skaitinės analizės nuoseklieji ir lygiagretieji algoritmai, kurie leis modeliuoti temperatūros pasiskirstymą elektos kabeliuose, optimizuoti jų geometrinius parametrus, modeliuoti metalų kaitinimo lazeriu medžiagos pašalinimo procesus.

Darbo rezultatų praktinė reikšmė. Dalis šio darbo medžiagos surinkta dalyvaujant Europos tyrimų, plėtros ir bendradarbiavimo programos EUREKA projekte E!3691 OPTCABLES „*Elektros saugiklių ir laidų išsidėstymo kabelių pluoštuose optimizavimas*“, dalyvavimo trukmė 2006 09–2009 12, projekto vadovas – prof. habil. dr. R. Čiegis.

Tyrimų rezultatai buvo panaudoti Lietuvos Aukštųjų technologijų projekte GRIDGLOBOPT „*Globalus sudėtingų sistemų optimizavimas naudojant didelio našumo skaičiavimus ir GRID technologijas*“, projekto vadovas – prof. habil. dr. R. Čiegis.

Abliacijos tyrimai, atlikti disertacijos rengimo metu, buvo naudojami vykdant Lietuvos Aukštųjų technologijų projektą FEMTOAPDIRBIMAS „*Lazerinis mikroapdirbimas ir prototipavimas didelio pasikartojimo dažnio femtosekundiniais impulsais*“, dalyvavimo trukmė 2007 04–2009 12, vadovas prof. habil. dr. V. Sirutkaitis (Vilniaus universiteto fizikos fakultetas).

Ginamieji teiginiai

1. Sukurti šilumos laidumo kompozicinėse medžiagose matematiniai modeliai, jų skaitinės analizės nuoseklieji ir lygiagretieji algoritmai, leidžiantys apskaičiuoti temperatūros pasiskirstymą laidų pluošte.

2. Lygiagretusis optimizavimo algoritmas, kuris remiasi variantų perrinkimo ir godžiosiomis strategijomis, taikytinas geometriniams laidų parametrams mažinti.

3. Skaitinės analizės nuoseklusis skaičiavimo algoritmas dviejų temperatūrų hiperboliniam modeliui taikytinas skaičiuojant pradines abliacijos fazes su įvairiomis relaksacijų trukmėmis.

Darbo rezultatų aprobavimas. Tyrimai atlikti Vilniaus Gedimino technikos universitete. Tyrimo rezultatai paskelbti 6-iuose moksliniuose straipsniuose. Penki straipsniai publikuoti recenzuojamuose mokslo leidiniuose: keturi – leidiniuose įtrauktuose į MII *Web of Science* duomenų bazę; vienas – leidinyje įtrauktame į *MII Conference Proceedings Citation Index Web of Science* duomenų bazę. Disertacijos rezultatai pristatyti 5-iose tarptautinėse ir

7-iose respublikinėse konferencijose, Vilniaus Gedimino technikos universiteto Matematinio modeliavimo katedros vykstančiuose seminaruose, Vilniaus universiteto, Matematikos ir informatikos instituto seminaruose. Tyrimų rezultatai gauti dalyvaujant trijose doktorantų vasaros mokyklose (2007 m Druskininkuose; 2008 m Suomijoje; 2009 m Austrijoje)

Disertacijos struktūra. Disertacijos aiškinamąjį raštą sudaro įvadas, trys skyriai, išvados, literatūros sąrašas. 1-ajame skyriuje pateikta šiluminių procesų lazerinėse ir elektroterminėse technologijose skaitinio modeliavimo uždavinių apžvalga. 2-ajame skyriuje pasiūlyti šilumos laidumo elektros kabeliuose cilindrinėje ir stačiakampėje srityse matematiniai modeliai ir jų skaitinės analizės nuoseklieji ir lygiagretieji algoritmai. Geometriniams laidų parametrams mažinti suformuluotas optimizavimo algoritmas ir pateiktas lygiagretusis optimizavimo algoritmas. 3-ajame skyriuje pateikta lazeriu kaitinamo metalo matematiniai modeliai, hiperbolinio matematinio modelio skaitinės analizės algoritmas, kaitinamos medžiagos dujų dinamikos modelis. Darbo apimtis yra 105 puslapiai, kuriuose pateikta: 142 formulės, 16 paveikslų ir 10 lentelių. Disertacijoje remtasi 145 kitų autorių literatūros šaltiniais.

Bendrosios išvados

Disertacijoje nagrinėjamiems realių technologinių procesų optimalumo uždaviniams spręsti (įrenginio masės mažinimo, medžiagos su minimaliomis pažeidomis apdirbimo) sukurti virtualaus eksperimentinio modeliavimo metodai ir įrankiai.

1. Elektros laidų pluoštų optimizavimo uždaviniui spręsti buvo realizuoti šie matematinio modeliavimo etapai:

- Pasiūlyti keli išsamūs ir supaprastinti dvimačiai kompozicinių medžiagų matematiniai modeliai, įvertinantys pagrindinius procesus, vykstančius nagrinėjamose medžiagose, leidžia apskaičiuoti temperatūros pasiskirstymą cilindrinės ir stačiakampės formos laidininkuose.
- Sudarytiems matematiniams modeliams sukurti ir ištirti stabilūs skaitiniai nuoseklieji ir lygiagretieji algoritmai, pasiūlyti modelių nežinomų parametrų identifikavimo būdai. Skaičiavimo eksperimentų rezultatų palyginimas su realiais eksperimentiniais duomenimis parodė, kad modeliai yra adekvatūs ir tinkami laidų pluoštų geometriniams parametrams optimizuoti.
- Sukurtas lygiagretusis optimizavimo algoritmas (šeimininkas – darbininkai ir duomenų lygiagretumo versijos) leidžia tiesioginį uždavinį spręsti daug kartų, todėl naudojant variantų perrinkimo metodus ir godžiąsias strategijas galima efektyviai (nuo 5 iki 20 proc.) sumažinti bendrą laidų masę įrenginyje.

- Sukurtas optimizavimo algoritmas gali būti taikomas mišrios architektūros procesoriams ir kitiems kelių lygių algoritmams realizuoti.

2. Metalų abliacijos matematinio modeliavimo uždaviniams spręsti buvo gauti tokie rezultatai:

- Metalą veikiant ultratrumpuoju lazerio impulsu šilumos perdavimo ir hidrodinaminės abliacijos procesai vyksta skirtingais laiko masteliais. Naudojant sukurtų ir ištirtų šių procesų (metalų kaitinimo, lydymosi ir garavimo) atskirus matematinius modelius ir jų skaitinės analizės algoritmus galima paprastai nusakyti abliacijos gylį nuo impulsų trukmės, energijos tankio ir skersinio energijos tankio pasiskirstymo.
- Klasikinis Furjė dėsnis neįvertina šilumos relaksacijos etapo, kuris tampa svarbiu, kai nagrinėjamų procesų laiko trukmės tampa mažos. Hiperbolinio dviejų temperatūrų modelio (kuriame įvertinamos šilumos relaksacijos trukmės) ištirti skaitiniai metodai ir jų algoritmai (kurių stabilumas nepriklauso nuo relaksacijos parametro) leidžia apskaičiuoti temperatūros pasiskirstymą (pradinę abliacijos fazę) pasirenkant įvairias relaksacijos parametro reikšmes.

Trumpos žinios apie autorę. Gerda Jankevičiūtė gimė 1979 m. gegužės 10 d. Utenoje. 2001 m. įgijo matematikos bakalauro laipsnį Kauno technologijos universitete Fundamentaliųjų mokslų fakultete. 2003 m. baigė Taikomosios matematikos magistrantūros studijų programą ir įgijo matematikos magistro kvalifikacinį laipsnį Kauno technologijos universitete Fundamentaliųjų mokslų fakultete.

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MATHEMATICAL MODELLING OF THERMAL PROCESSES IN LASER AND ELECTROTHERMAL TECHNOLOGIES

Summary of Doctoral Dissertation
Physical Sciences, Mathematic (01P)

Gerda JANKEVIČIŪTĖ

ŠILUMINIŲ PROCESŲ LAZERINĖSE IR ELEKTROTERMINĖSE TECHNOLOGIJOSE MATEMATINIS MODELIAVIMAS

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