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THE NUMERICAL ANALYSIS OF NONLINEAR MATHEMATICAL MODELS ON GRAPHS

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Introduction

Problem Formulation

The numerical algorithms for non-stationary mathematical models in non-standard domains are investigated in the dissertation. Problem definition domain is represented by branching structures, which can be defined using the terminology of oriented graphs. Problems of transportation through the narrow pipes, modeling of electrical circuits and other may be considered on branching structures, and the neuron simulation models are the most widely applied problems of such type.

Because of the special geometry of the neurons, when the length of the segments of a cell is hundreds times bigger than its diameter, locally one-dimensional models are applied. During construction of numerical approximations of reaction-diffusion systems on branched structures, very important problems arise due to approximation of conjugation equations at branch points. Such models are often nonlinear and require additional calculations in order to represent the solution the system of linear equations. The structure and the amount of calculations significantly grow up when groups of cells connected by lots of synaptic connections are modeled. Computation needed to fit the mathematical model to experimental data by exhaustively exploring the parameter space also grows exponentially with the number of parameters. Therefore, there is a need to solve effectively these problems and one of the options is the parallelization of the algorithms.

The problem of the identification of nonlinear model is often challenging not only due to the amount of computations, but also due to the choice of the optimization algorithm and the limited facilities of parameters identifiability.

The parabolic or elliptic problems can be formulated not only in non-standard domains, but also with non-classical boundary conditions. During recent decades the nonlocal problems for partial differential equations are actively investigated. Instead of classical boundary conditions the relationships between the solution and its derivatives on the boundary of the domain and inside the domain are used.

Topicality of the Research Work

The parabolic reaction-diffusion model on branching structure investigated in the dissertation represents a generalized model of cell excitation. The well known example of this kind of models is given by the nonlinear Hodgkin-Huxley action potential model. The problem is defined on the arbitrarily branching structure with two different conjugation equations at the branch points. The first one describes a conservation of the fluxes at vertexes, and the second conjugation condition defines the conservation of the current flowing at the soma in neuron models.

θ -implicit finite difference scheme and two predictor-corrector type finite difference schemes are investigated. The stability and convergence of the discrete solution is proved, sequential algorithms are implemented and parallelized, the ef-

efficiency and scalability analysis of the parallel algorithms is given.

The numerical analysis of classical parabolic problem becomes complicated not only in non-standard domains, but also in the case of non-classical boundary conditions. During recent decades problems with nonlocal boundary conditions are actively investigated because of theoretical interest and also due to the practical need: many physical, chemical, biological and ecological processes are described by mathematical models with nonlocal conditions. The numerical analysis of one-dimensional parabolic problem with one class of nonlocal integral boundary conditions is presented in the dissertation, the stability and convergence of the discrete scheme is proved.

While investigating the nonlinear model of excited carrier decay in a semiconductor the apriori estimates of the solution of differential problem is proved, the analysis of linearized finite-difference scheme and fitting of nonlinear model to the experimental results are performed.

Research Object

The main research objects of the dissertation are the numerical methods for modeling of processes on branching structures, the stability and convergence of obtained discrete schemes, parallel implementation of these algorithms; the stability and convergence of the discrete schemes approximating nonlocal boundary conditions; problem of the identification of the nonlinear model.

The Aim of the Work

The aim of the dissertation is to construct and implement the numerical algorithms for parabolic problems in non-standard domains or with non-classical boundary conditions, to investigate the stability and convergence of obtained schemes; to implement the parallel versions of these algorithms and investigate the efficiency and scalability of parallel versions; to investigate the nonlinear model identification problem.

Tasks of the Work

To achieve the aim of the work the following tasks are set:

1. To construct and investigate the efficient finite-difference schemes for linear parabolic problem on branching structure with different flux conservation equations defined at the branch points.
2. To develop and investigate the parallel versions of the sequential finite-difference schemes and perform the numerical experiment of neuron simulation.
3. To perform the numerical analysis of parabolic problem with one class of nonlocal integral boundary conditions and investigate the influence of signs of coefficients in the nonlocal condition on the stability and conver-

gence of the discrete solution.

4. To perform the numerical analysis of the nonlinear model of excited carrier decay in a semiconductor. Carry out the model identification experiment.

Applied Methods

The numerical methods for partial differential equations and techniques for investigation of their stability and convergence, methods of applied functional analysis, methods of constructing and investigation of parallel algorithms, global optimization methods and methods of parameter identifiability analysis for nonlinear mathematical models are applied in this study. The programs for numerical experiments are written in C++ using MPI library for parallel versions of codes and software package *Metis* is used for graph partitioning; some numerical results are compared with the results obtained with NEURON simulation environment.

Scientific Novelty

A significant part of the dissertation is dedicated to the linear parabolic model on graphs, since the models of neuron excitation are conditionally linear and can be decomposed into several linear systems. There are many scientific publications on the numerical methods for the models of neuron excitation, but their stability and convergence is proved only for one-dimensional case. Two flux conservation equations at the branch points are studied in the dissertation, the methods for the numerical analysis of boundary conditions of second and third type are applied for the numerical analysis of flux equations. Besides the traditional for this type of problems θ -implicit finite difference scheme, two predictor-corrector type finite difference schemes are investigated. The stability and conditional convergence of these schemes is proved. It is also proved, that the efficiency of the parallel implicit finite difference scheme employing the "exact domain decomposition" is sufficiently high, and this scheme can be successfully used in parallel computations. The non-iterative linearized discrete scheme is proposed and studied for the nonlinear model of excited carrier decay, the model identification problem is considered.

The problem with nonlocal integral boundary condition is also considered in the dissertation. The systematic analysis of this class of nonlocal conditions is performed in the plane of parameters (a, b) . The stability analysis of the implicit Euler scheme is performed in the maximum norm, the known stability results are improved. In case of pure integral condition the estimate of the discrete problem sensitivity to the integral condition is proved, showing the conditional convergence of the scheme, and the regularization relation between discrete steps is suggested.

Practical Value of the Work Results

The numerical algorithms for reaction – diffusion problems on branching structures are implemented. The parallel versions of algorithms employing data distribution paradigm are implemented for large simulations.

The optimization algorithm for the nonlinear model of excited carrier decay in a semiconductor is implemented. The results of model parameter identifiability analysis indicate, that some parameters are unidentifiable.

Statements Presented for Defence

1. The analysis methods for discrete mathematical models with boundary conditions of the second and the third type are applicable for the analysis of discrete mathematical models on graphs.
2. The efficiency of implemented parallel algorithms mostly depends on data partitioning quality and memory bus saturation when 2 or 4 cores per node are used.
3. The stability and convergence of the discrete scheme for one-dimensional parabolic problem with nonlocal integral boundary condition depends on the parameters of nonlocal condition.
4. The discrete solution of the nonlinear model of excited carrier decay mimics the main properties of the solution of ODE. The identifiability of model parameters with experimental data used in calculations is limited.

Approval of the Work Results

The research is performed at the Vilnius Gediminas Technical University. The results of the dissertation are published in 7 publications, 6 of them in the reviewed scientific journals. The results were presented at 13 Lithuanian and international conferences and 4 seminars at the Department of Mathematical Modeling of Vilnius Gediminas Technical University.

The Scope of the Scientific Work

The dissertation consists of an introduction, 5 chapters, main conclusions, bibliography and the list of the author's publications. The first chapter presents the overview of mathematical models in non-standard domains or with non-classical boundary conditions. The second chapter presents three numerical algorithms for the linear parabolic problems on branching structures and the stability and convergence analysis of these algorithms. The third chapter presents the parallel versions of the algorithms, the efficiency and scalability analysis of parallel algorithms, and the numerical experiments of the excitation of neuron. The fourth chapter deals with one-dimensional parabolic problem with nonlocal integral boundary condition. The implicit discrete scheme is presented, the stability and convergence analysis of the scheme is performed systematically for a class of parameters (a, b)

of nonlocal condition. In chapter five the nonlinear model of excited carrier decay in a semiconductor is presented. The apriori estimate of the differential solution is proved, the analysis of the linearized numerical scheme and the results of the model fitting experiment using genetic algorithm are presented.

1. Mathematical Models in Non-Standard Domains or With Non-Classical Boundary Conditions

The review on mathematical models on branching structures and problems with nonlocal boundary conditions is given in the first chapter.

Mathematical Models on Graphs: the Models of Neuron Excitation. The best-known models, described by reaction – diffusion – transportation equations on branching structures are given by neuron simulation models, which are based on the Hodgkin-Huxley (HH) nonlinear system:

$$C_m \frac{\partial V}{\partial t} = \frac{a}{2R_a} \frac{\partial^2 V}{\partial x^2} - R(V), \quad (1)$$

$$R(V) = \bar{g}_K n^4 (V - V_K) + \bar{g}_{Na} m^3 h (V - V_{Na}) + \bar{g}_l (V - V_l), \quad (2)$$

$$\frac{dn}{dt} = \alpha_n(V)(1 - n) - \beta_n(V)n, \quad (3)$$

$$\frac{dm}{dt} = \alpha_m(V)(1 - m) - \beta_m(V)m, \quad \frac{dh}{dt} = \alpha_h(V)(1 - h) - \beta_h(V)h.$$

The model adapted for one segment of giant squid axon became the foundation for the whole modern theory of action potential in excitable cell. FitzHugh (1961) proposed the simplified model, facilitating the understanding of action potential generation, which is widely used for simulation of groups of cells. These models served as a framework for other models of excitation, for instance, Morris-Lecar, Hindmarsh-Rose, etc.

The well-known property of models of excitation is their conditional linearity. The voltage equation (1) is linear, if gating variables m, n and h are known. On the other hand, equations (3) are linear, the value of voltage V is known. The property of the conditional linearity allows to separate the initial nonlinear problem into two linear ones, which can be solved using Picard iterations. Mascagni (1990) proved the convergence of the implicit Euler method with Picard iterations for the Hodgkin-Huxley equations in L_2 norm for sufficiently small values of the time discrete step. Chiegis (1992) proved the stability and convergence of the Crank-Nicolson scheme for a class of models of excitation. The stability and convergence of the implicit Euler method with Picard iterations in maximum norm is also proved in this work.

Typically neurons have a large number of long extensions called dendrites, also the axons often are of tree-like structure. These segments can be studied as

an extensively branched structures, where each cable segment is defined by its diameter and membrane properties.

The most popular method for discretizing the branched structure was proposed by Rall (1964). It is called the compartmental modeling method and it is based on the discretizing the whole structure into small parts, whose membranes are isopotential. The changes of membrane physical properties and action potential changes appears not inside the sections, but between them. This method is employed by the most popular environments for neuronal modeling, including NEURON (Hines, Carnevale 1997) and GENESIS (Bower, Beeman 1998).

The system of equations obtained after discretizing the problem on branched structure is no more tridiagonal because of branch points. Special methods for solving this kind of systems must be applied, especially for big size real-world problems. Hines (1984) proposed the method for the tree-like structures without the closed loops. The point is the special algorithm for enumerating branches, which gives the liner system matrix of a special form, this matrix is solved in $\mathcal{O}(N)$ operations, where N is the number of points in the discrete grid.

Mascagni (1991) proposed algorithm, employing "the exact decomposition". The reaction – diffusion equations are approximated using implicit Euler scheme, then using the modified forward factorization algorithm the solution on branches is expressed as a sum of solutions at branch points. Substituting these solutions into discrete flux conservation equations a reduced system of linear equations is obtained, whose size equals to the number of connections of different compartments.

Rempe, Chopp (2006) proposed predictor-corrector finite difference scheme for Hodgkin-Huxley model on branching structures. Equations on different edges of the graph are decoupled into one-dimensional problems, which are efficiently computed using factorization algorithm. The complexity of this algorithm is only $\mathcal{O}(N)$.

Nonlocal Boundary Conditions. Problems with nonlocal boundary conditions nowadays are actively studied in heat conduction and thermodynamics, plasma physics and others. A class of the problems with integral conditions can be distinguished among other nonlocal conditions. The nonlocal integral boundary conditions are interpreted as a generalization of nonlocal conditions. The investigations of partial differential problems with integral boundary conditions were started by Cannon (1963) and continued by Čiegis (2006), Day (1983), Dehghan (2005), Ekolin (1991), Pečiulytė *et al* (2005), Sapagovas (2005) and many other authors. The area of differential problems with nonlocal boundary conditions is very wide, and only separate, though very important cases are studied thoroughly.

2. Parabolic Problem on Graph

The linear parabolic problem on branched structure is studied in the second chapter. Let $P = \{p_j, j = 1, \dots, J\}$ be a set of branching points. Some of these points are joint by individual edges making a set of edges $E = \{e_k = (p_{k_s}, p_{k_f}), p_{k_s}, p_{k_f} \in P, k = 1, \dots, K\}$, where p_{k_s} is a starting point of edge e_k , and p_{k_f} is an end point of the same edge. Let $l_k = |e_k|$ be a length of e_k , and let x be a distance along the interval $(0, l_k)$, which defines the given edge in the geometrical domain. The given graph is oriented, this property is required for formulation of conservation equations at vertexes of the graph. For each point $p_j \in P$ we denote the sets of edges going in and out of point, respectively:

$$N^+(p_j) = \{e_k : e_k = (p_{j_s}, p_j) \in E, s = 1, \dots, S_j\},$$

$$N^-(p_j) = \{e_k : e_k = (p_j, p_{j_f}) \in E, f = 1, \dots, F_j\}.$$

On the graph (E, P) we consider a system of parabolic linear problems for functions $\{u^k(x, t)\}$:

$$\frac{\partial u^k}{\partial t} = \frac{\partial}{\partial x} \left(d^k \frac{\partial u^k}{\partial x} \right) - q^k u^k + f^k, \quad 0 < x < l_k, \quad k = 1, \dots, K, \quad (4)$$

$$0 < d_0 \leq d^k(x, t) \leq d_M, \quad q^k(x, t) \geq 0, \quad f^k = f^k(x, t), \quad (5)$$

$$u^k(x, 0) = u_0^k(x) \quad 0 < x < l_k, \quad k = 1, \dots, K. \quad (6)$$

Let us divide all branch points into three sets $P = T \cup P_1 \cup P_2$, consisting of the termination points T and branch points of the first and second type. The point is assigned to a set T if there exists only one edge, which terminates at the given point: $T = \{p_j : p_j \in P, N^+(p_j) = \emptyset \text{ or } N^-(p_j) = \emptyset\}$. Boundary conditions of the first type are given at the termination points.

Two flux conservation equations are given at the branch points of the first and the second type:

$$\sum_{e_k \in N^+(p_j)} d^k \frac{\partial u^k}{\partial x} \Big|_{x=l_k} = \sum_{e_m \in N^-(p_j)} d^m \frac{\partial u^m}{\partial x} \Big|_{x=0}, \quad \forall p_j \in P_1, \quad (7)$$

$$c \frac{\partial u_s}{\partial t} + q_s u_s = \sum_{e_m \in N^-(p_s)} d^m \frac{\partial u^m}{\partial x} \Big|_{x=0} - \sum_{e_k \in N^+(p_s)} d^k \frac{\partial u^k}{\partial x} \Big|_{x=l_k} + f_s, \quad \forall p_s \in P_2. \quad (8)$$

The continuity constraints are satisfied at all vertexes of the graph:

$$u^m(p_j, t) = u^k(p_j, t), \quad \forall p_j \in P_1, \quad e_m, e_k \in N^\pm(p_j), \quad (9)$$

$$u_s(t) = u^m(p_s, t), \quad \forall p_s \in P_2, \quad e_m \in N^\pm(p_s).$$

The Implicit Scheme. Using the θ -method, differential equations (4) are ap-

proximated by the finite difference equations with parameter $\theta \in [0, 1]$. We prove, that the discrete problem has a unique solution. The stability and convergence of this scheme is studied in L_2 , H_1 and L_∞ norms. The maximum principle is applied to show unconditional stability of the discrete scheme, though it is not suitable to evaluate precisely the convergence rate. Using the energy estimate method the stability and convergence in L_2 norm are proved, when $\theta \in [\frac{1}{2}, 1]$:

$$\|U^n - u^n\| \leq C\sqrt{t^n}(\tau^{\sigma_\theta} + h^2),$$

where $\sigma_\theta = 2$, if $\theta = 1/2$, otherwise $\sigma_\theta = 1$. The proved rate of convergence in H_1 norm is

$$|U^n - u^n|_1 \leq C\sqrt{t^n}(\tau^{\sigma_\theta} + h^{3/2}).$$

Using the technique of bounding functions and comparison theorems the convergence rate for fully implicit scheme ($\theta = 1$) in L_∞ norm is proved:

$$\|U^n - u^n\|_\infty \leq C(\tau + h^2).$$

The results of numerical experiment confirm the convergence rate $\mathcal{O}(\tau^{\sigma_\theta} + h^2)$.

Predictor-Corrector Algorithm I. The predictor-corrector splitting and domain decomposition methods are widely used to speed-up calculations by applying parallel algorithms. We investigate two finite difference predictor-corrector schemes based on different domain decomposition. The first scheme is obtained by dividing some edges of the graph, therefore a set of problems on sub-graphs is obtained and these subproblems can be solved efficiently in parallel:

1. **Graph decomposition step.** During the first step the problem domain is decomposed into subdomains. Each grid on the edges, which connect vertices belonging to different subdomains, is divided into two subgrids by midpoints.
2. **Predictor step.** The new values of the solution at the splitting points are computed in parallel. The explicit Euler approximation is used to discretize the differential equation (4).
3. **Domain decomposition step.** Solutions on each subgraph are computed in parallel using the implicit finite difference scheme. The predicted values are used as the interface boundary conditions.
4. **Corrector step.** The values of the solution at the splitting points are updated in parallel using the implicit finite difference scheme.

Using the energy estimates method the unconditional stability of the discrete scheme in the special energy norm is proved. It is important to note, that only conditional convergence can be proved in this norm:

$$\|U^n - u^n\|_E \leq Ct^n \left(\tau + h^{\frac{3}{2}} + \frac{\tau\sqrt{\tau}}{h} \right).$$

Solving the simplified one-dimensional problem the convergence estimate in the maximum norm is proved:

$$\|U^n - u^n\|_\infty \leq C\left(\tau + h^2 + \frac{\tau^2}{h}\right).$$

It is shown in dissertation, that the presented algorithm can be written as Douglas type scheme, based on the domain decomposition method. For a simple case of one dimensional parabolic problem, the convergence analysis is done by using results from (Vabishchevich 2011). The optimality of asymptotical error estimates is investigated. The presented results of numerical experiment confirm the estimate of the splitting error $\mathcal{O}\left(\frac{\tau^2}{h}\right)$.

Predictor-Corrector Algorithm II. The second predictor-corrector algorithm is based on the decomposition of the problem into simple one-dimensional problems on each edge, which can be efficiently solved by factorization algorithm:

1. **Predictor step.** The solution values at the branch points $p_j \in P_1 \cup P_2$ are calculated by using the explicit Euler approximation of the flux conservation equations.
2. **Domain decomposition step.** The solutions on edges are calculated using factorization algorithm. The predicted values are used as the interface boundary conditions.
3. **Corrector step.** The solution values at the branch points $p_j \in P_1 \cup P_2$ are updated by using the implicit Euler approximation of the flux conservation equations.

The second predictor-corrector algorithm is also proved to be unconditionally stable in special energy norm, but its convergence in the related norm is conditional. Presented results of numerical experiment show the same splitting error estimate $\mathcal{O}\left(\frac{\tau^2}{h}\right)$.

3. Parallel Algorithms

The parallel versions of the implicit algorithm and both predictor-corrector algorithms are developed in the third chapter. All parallel algorithms are based on data distribution paradigm.

The descriptions of three parallel algorithms, the estimates of their complexity, theoretical efficiency and scalability are given in the dissertation. Theoretical estimates show, that the efficiency of the algorithms mainly depends on domain partition quality and negative effects of global memory usage by cores (bottleneck effect).

Computations were performed on Vilkas cluster of computers at Vilnius Gediminas Technical University, consisting of nodes with Intel®Core™ processor i7-860 @ 2.80 GHz and 4 GB DDR3-1600 RAM. Each of the four cores can complete

Table 1. Performance results for the parallel Crank-Nicolson solver for the Hodgkin-Huxley model

$p(n \times c)$	1×2	2×1	1×4	2×2	4×1	2×4	4×2	8×1	4×4	8×2	8×4
$T_0 = 947$											
T_p	478	470	273	240	235	138	121	114	69	63	34
S_p	1.98	2.01	3.47	3.95	4.03	6.86	7.83	8.31	13.7	15.0	27.9
E_p	0.99	1.01	0.87	0.99	1.01	0.86	0.99	1.04	0.86	0.94	0.87

up to four full instructions simultaneously. The results of numerical experiments confirm theoretical estimates.

The numerical simulation of neuron excitation based on the Hodgkin-Huxley model is given in this chapter. The obtained performance results for the parallel Crank-Nicolson solver are presented in Table 1. Here for each number of processors $p = n \times c$, where n denotes the number of nodes and c the number of cores per node, the coefficients of the algorithmic speed up $S_p = T_0/T_p$ and efficiency $E_p = S_p/p$ are presented. T_p denotes the CPU time required to solve the problem by using p processors. The results confirm good efficiency of the parallel algorithm.

4. Parabolic Problem with Nonlocal Integral Boundary Condition

Parabolic problem with nonlocal integral boundary condition is studied in the forth chapter:

$$\frac{\partial u}{\partial t} = \frac{\partial}{\partial x} \left(d(x) \frac{\partial u}{\partial x} \right) - q(x)u(x) + f(x), \quad 0 < x < 1, \quad t > 0, \quad (10)$$

$$u(0, t) = \mu_0, \quad au(1, t) + b \int_0^1 \gamma(x)u(x, t)dx = g(t), \quad t > 0, \quad (11)$$

$$u(x, 0) = u_0(x), \quad 0 \leq x \leq 1, \quad (12)$$

$$0 < d_0 \leq d(x) \leq d_M, \quad q(x) \geq 0, \quad \gamma(x) \geq 0.$$

The differential problem is approximated by the implicit Euler scheme, the integral condition is approximated using trapezoid rule. Three cases of the coefficients (a, b) are studied:

1. Coefficients $a = 1, b = -1$. For sufficiently small parameter $\gamma(x) \leq \gamma_M$ it is proven, that the discrete problem has the unique solution, which converges to the solution of differential problem (10) – (12), and the following estimates are valid:

$$|u(x_j, t^n) - U_j^n| \leq C(\tau + h^2), \quad (x, t) \in \bar{\omega}_h \times \omega_\tau.$$

2. Coefficients $a = 1, b = 1$. For bounded $\gamma(x) \leq \tilde{\gamma}_M$ it is proven, that, when the real parts of eigenvalues of the discrete operator are nonnegative, the discrete problem has the unique solution, which converges to the solution of differential problem (10) – (12), and the following estimates are valid:

$$|u(x_j, t^n) - U_j^n| \leq C(\tau + h^2), \quad (x, t) \in \bar{\omega}_h \times \omega_\tau.$$

3. Coefficients $a = 0, b = 1$. When the real parts of eigenvalues of the discrete operator are nonnegative, the sensitivity estimate of the discrete problem to the integral condition was proved, resulting the conditional convergence in general:

$$|u(x_j, t^n) - U_j^n| \leq Ct^n(\sqrt{\tau} + \frac{h^2}{\sqrt{\tau}}) \quad (x, t) \in \bar{\omega}_h \times \omega_\tau.$$

A regularization of the discrete scheme is suggested by putting a relation between the discrete steps. When function $g(t)$ is continuous, a regularization of the discrete scheme can be done by differentiating the boundary condition:

$$Tu := \frac{\partial}{\partial t} \int_0^1 \gamma(x) u(x, t) dx = g'(t).$$

5. Model of Excited Carrier Decay

The nonlinear mathematical model of excited carrier decay in a semiconductor is investigated in the fifth chapter:

$$\frac{dn}{dt} = I_L(t) - \sigma_n^t v_{th}^n n(N_t - n_t) + e_n^t n_t - \sigma_n^r v_{th}^n n(N_r - n_r) + e_n^r n_r - \frac{n}{\tau_0}, \quad (13)$$

$$\frac{dn_t}{dt} = \sigma_n^t v_{th}^n n(N_t - n_t) - e_n^t n_t, \quad (14)$$

$$\frac{dn_r}{dt} = \sigma_n^r v_{th}^n n(N_r - n_r) - e_n^r n_r - \sigma_p^r v_{th}^p p n_r + e_p^r (N_r - n_r), \quad (15)$$

$$\frac{dp}{dt} = I_L(t) - \sigma_p^r v_{th}^p p n_r + e_p^r (N_r - n_r) - \frac{p}{\tau_0}, \quad (16)$$

$$n(0) = 0, \quad n_t(0) = 0, \quad n_r(0) = 0, \quad p(0) = 0, \quad (17)$$

where n is the electron concentration, p is the hole concentration, n_t and n_r are the concentrations of electrons, occupying the trap level and recombination center, respectively. σ represents the capture cross section for the electrons (n) or holes (p), where superscript t means trap property and r means recombination center property. N_t and N_r are the concentrations of the trap and recombination center, v_{th} is thermal velocity of the carriers, τ_0 is the lifetime of free carriers. $I_L = I_0 \exp\left(-\left(\frac{t-\Delta}{\Delta/2}\right)^2\right)$ is electron generation by the laser pulse from the valence band.

The emission coefficients e are related to the capture cross section values by the equations

$$\begin{aligned} e_n^t &= \sigma_n^t v_{th} N_c \exp\left(-\frac{E_t}{kT}\right), & e_n^r &= \sigma_n^r v_{th} N_c \exp\left(-\frac{E_r}{kT}\right), \\ e_p^r &= \sigma_p^r v_{th} N_v \exp\left(-\frac{E_g - E_r}{kT}\right), \end{aligned}$$

where E indicates the energy levels of the trapping center, recombination center and the bandgap, T is temperature, N_c and N_v are effective density of states for conduction and valence band.

The apriori estimate of the solution of differential problem (13)–(17) is proved:

$$0 \leq n(t) \leq C_n, \quad 0 \leq n_t(t) \leq N_t, \quad 0 \leq n_r(t) \leq N_r, \quad 0 \leq p(t) \leq C_p,$$

where the constants

$$C_n = \tau_0(I_0 + e_n^t N_t + e_n^r N_r), \quad C_p = \tau_0(I_0 + e_p^r N_r).$$

The analysis is performed for the linearized backward Euler method, as a good starting point to construct more accurate and robust numerical solvers. For sufficiently smooth solution of differential problem (13)–(17) it is proven, that there exists a constant $C = C(M, t^k)$ such that the estimate holds

$$\|Z^k\| \leq C\tau, \quad k = 1, 2, \dots, K,$$

where Z^k defines the global error of the discrete solution:

$$\|Z^k\| = \max(|z_n^k|, |z_{n_t}^k|, |z_{n_r}^k|, |z_p^k|).$$

The model identification problem is also considered in this chapter. A genetic algorithm (GA) was chosen for the calculations. Compared to the gradient-based optimization methods, genetic algorithms are more suitable, when optimized function is discontinuous, nonlinear or/and is notorious for other complexities. The fitness of the individual is evaluated using the least squares method.

The activity of the deep center in the bandgap is defined by the carrier capture cross sections σ and concentration of the center N . When one trapping center and one recombination center is considered, the involved parameters vector is $\theta = (\sigma_n^t, \sigma_n^r, \sigma_p^r, N_t, N_r)$. Applying sensitivity-based and experimental methods of parameter identifiability, the set of identifiable parameters $\theta = (\sigma_n^t, \sigma_n^r)$ is established.

The results of numerical calculations are given on Fig 1. The solution with the parameters set estimated by GA fits good the experimental data. This result is very close to the parameters values proposed by physics. However, in the manufacture of compensated semiconductors, parameters of the individual crystals can vary, so

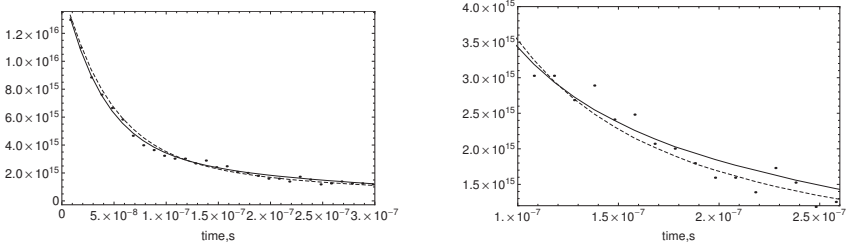


Fig 1. Electron decay $n(t)$: the solid curve corresponds to the calculation results for the parameters set proposed by physics, dashed curve – for the set identified by GA, dots – to the experimental data

the task of parameters identification can be raised even for sufficiently investigated materials.

Results and Conclusions

In this work, some parabolic problems on branching structures and problems with integral boundary conditions are investigated. The main results are the following:

1. For reaction-diffusion problems on branched structures the unconditional stability of θ -implicit finite difference scheme is proved, when parameter $\theta \in [\frac{1}{2}, 1]$. The convergence estimates obtained by classical maximum principle are improved, the convergence rate $\mathcal{O}(\tau + h^2)$ in the maximum norm is proved for fully implicit scheme. Theoretical results are confirmed by numerical experiments.
2. The analysis of two predictor-corrector type discrete schemes is performed by the energy estimates method. It was proven, that both schemes are unconditionally stable, though their convergence in related norm is only conditional because of the splitting error. Employing the equivalence of predictor-corrector and Douglas splitting schemes, new stability estimates are obtained. The analysis of simplified one-dimensional problem and the results of numerical experiments show the splitting error estimate $\mathcal{O}(\tau^2/h)$.
3. The parallel versions of algorithms are implemented. The given theoretical efficiency and scalability analysis of the parallel algorithms and the results of numerical simulations show good scalability (linear for predictor-corrector schemes and quadratic in the worst case for fully implicit scheme). It is proven, that the efficiency reduction occurs mainly due to the memory bus saturation when 2 or 4 cores per node are used.
4. The numerical analysis of parabolic problem with one class of integral

boundary conditions is performed. It is proven, that the stiffness and convergence of the discrete implicit scheme depends on the signs of coefficients in the nonlocal boundary condition. The known stability results are improved. In the case of a pure integral boundary condition the conditional convergence is proved and the regularization relation between discrete time and space steps is proposed.

List of Scientific Publications on the Topic of Dissertation

In the Reviewed Scientific Journals

Tumanova, N.; Čiegis, R. 2012. Predictor-corrector domain decomposition algorithm for parabolic problems on graphs. *Mathematical Modelling and Analysis*, 17(1): 113–127. ISSN 1392-6292 [ISI Web of Science].

Čiegis, R.; Tumanova, N. 2012. Stability Analysis of Implicit Finite-Difference Schemes for Parabolic Problems on Graphs. *Numerical Functional Analysis and Optimization*, 33(1): 1–20. ISSN 0163-0563 [ISI Web of Science].

Čiegis, R.; Tumanova, N. 2010. Numerical solution of parabolic problems with nonlocal boundary conditions. *Numerical Functional Analysis and Optimization*, 31(12): 1318–1329. ISSN 0163-0563 [ISI Web of Science].

Čiegis, R.; Tumanova, N. 2010. Parallel predictor-corrector schemes for parabolic problems on graphs. *Comp. Meth. Appl. Math.*, 10(3): 275–282. ISSN 1609-4840.

Čiegis, R.; Tumanova, N. 2010. Finite-difference schemes for parabolic problems on graphs. *Lithuanian Mathematical Journal*, 50(2): 164–178. ISSN 0363-1672 [ISI Web of Science].

Pincevičius, A.; Meilūnas, M.; Tumanova, N. 2007. Numerical simulation of the conductivity relaxation in the high resistivity semiconductor. *Mathematical Modelling and Analysis*, 12(3): 379–388. ISSN 1392-6292 [ISI Web of Science].

In Other Scientific Works

Tumanova, N. 2008. Netiesiniai modeliai grafuose. *II-osios Lietuvos jaunųjų mokslininkų konferencijos „Mokslas – Lietuvos ateitis“, įvykusios 2008 m. kovo 28 d. Vilniuje, pranešimų medžiaga*, 193–200. ISBN 978-9955-28-300-3.

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NETIESINIŲ MATEMATINIŲ MODELIŲ GRAFUOSE SKAITINĖ ANALIZĖ

Problemos formulavimas

Darbe nagrinėjami paraboliniai modeliai nestandartinėse srityse arba su neklasikinėmis kraštinėmis sąlygomis. Matematinų modelių grafuose ypatumas yra uždavinio apibrėžimo sritis – matematinės lygtys formuluojamos šakotose struktūrose, kurios gali būti aprašomos pasitelkus grafų teorijos terminiją. Tokiose struktūrose yra formuluojami transportavimo siaurais vamzdžiais, elektros grandinės modeliavimo ir kiti uždaviniai, tačiau plačiausiai žinomi ir tiriama modeliai šakotose struktūrose yra neurono sužadinimo modeliai.

Dėl neuronų geometrijos ypatumų, kai ląstelės segmentų ilgiai yra šimtus kartų didesni už skersmenis, taikomi lokaliai vienmačiai modeliai. Konstruojant reakcijos – difuzijos modelio šakotose struktūrose skaitinę aproksimaciją svarbiu uždaviniu tampa srautų tvermės dėsnių išsišakojimo taškuose skaitinė aproksimacija. Tokie modeliai dažnai pasižymi netiesinėmis savybėmis. Modeliuojant ląstelių, sujungtų sudėtingais sinapsiniais ryšiais, grupes, smarkiai didėja struktūra kartu su skaičiavimų apimtimi. Skaičiavimų apimtis taip pat sparčiai auga sprendžiant modelio identifikavimo uždavinį. Todėl atsiranda poreikis ieškoti būdų, kaip efektyviai spręsti tiesinės algebros uždavinius ir algoritmų lygiagretinimas yra vienas iš sprendimo variantų.

Netiesinio modelio identifikavimo uždavinys dažnai yra iššūkis ne tik dėl didelės skaičiavimų apimties, bet ir dėl tinkamo optimizavimo algoritmo parinkimo bei ribotų parametrų identifikuojamumo galimybių.

Klasikiniai uždaviniai gali būti formuluojami ne tik nestandartinėse srityse, bet ir su neklasikinėmis kraštinėmis sąlygomis. Pastaraisiais dešimtmečiais aktyviai tiriama nelokalieji uždaviniai diferencialinėms lygtims dalinėmis išvestinėmis, kuriuose vietoje klasikinių kraštinių sąlygų naudojami sąryšiai tarp ieškomos funkcijos ir jos išvestinių ant srities kontūro ir srities viduje.

Darbo aktualumas

Disertacijoje nagrinėjamas vienmatis parabolinis reakcijos – difuzijos modelis šakotose struktūrose yra apibendrintas sužadinimo modelis, kurio vienas iš konkretesnių ir plačiausiai žinomų pavyzdžių yra Hodžkino ir Hakslio netiesinis modelis, aprašantis aksono sužadinimą. Uždavinys formuluojamas šakotose struktūrose su dviejų tipų tvermės dėsniais išsišakojimo taškuose. Šie dėsniai leidžia aprašyti kaip ir paprastą srautų persiskirstymą išsišakojimo taškuose, taip ir sudėtingesnę mazgą, kuriame vyksta reakcija. Antrasis tvermės dėsnis gali būti naudojamas aprašant somą neurono modelyje.

Tyrimų eigoje ištirtos svorinė ir dviejų tipų prediktoriaus ir korektoriaus baigtinių skirtumų schemos, aproksimuojančios matematinį modelį. Atlikta šių sche-

mų stabilumo ir konvergavimo analizė, sudaryti ir realizuoti algoritmai. Nuoseklieji algoritmai yra išlygiagretinti, pateikta lygiagrečiųjų algoritmų efektyvumo ir išplečiamumo analizė.

Klasikinio parabolinio uždavinio analizė tampa sudėtingesne ne tik nagrinėjant nestandartinę sritį, bet ir naudojant neklasikines kraštines sąlygas. Pastaraisias dešimtmečiais ypač aktyviai tiriamos nelokalios kraštinės sąlygos. Šių uždavinių tyrimai sąlygojami ne tik teorinio intereso, bet ir praktinės būtinybės: daug fizikinių, cheminių, biologinių procesų aprašomi diferencialinėmis lygtimis su nelokaliosiomis sąlygomis. Darbe atlikta parabolinio uždavinio su integraline kraštine sąlyga analizė, ištirtas skaičiavimo schemų stabilumas ir konvergavimas.

Nagrinėjant netiesinį sužadintų krūvininkų apšviestame puslaidininkyje rekombinacijos modelį įrodytas diferencialinio sprendinio apriorinis įvertis, atlikta linearizuotos schemas analizė, sprendžiamas netiesinio modelio parametrų nustatymo uždavinys.

Tyrimų objektas

Darbo tyrimo objektas yra skaitiniai metodai, skirti procesų modeliavimui šakotose struktūrose, sudarytų diskrečiųjų schemų stabilumas ir konvergavimas, jų pagrindu sudaryti lygiagretieji algoritmai; diskrečiųjų schemų, skirtų uždaviniams su nelokaliosiomis kraštinėmis sąlygoms aproksimuoti stabilumas ir konvergavimas; netiesinio modelio identifikavimo uždavinys.

Darbo tikslas

Disertacijos tikslas yra sudaryti ir realizuoti skaitinius algoritmus, skirtus paraboliniams uždaviniams nestandartinėse srityse arba su neklasikinėmis kraštinėmis sąlygomis spręsti, išnagrinėti sudarytų skaitinių schemų stabilumą ir konvergavimą; atlikti algoritmų lygiagretinimą ir ištirti lygiagrečiųjų algoritmų efektyvumą ir išplečiamumą; išnagrinėti netiesinio modelio identifikavimo uždavinį.

Darbo uždaviniai

Igyvendinant numatytus darbo tikslus buvo sprendžiami šie uždaviniai:

1. Sudaryti ir ištirti skaitinius algoritmus tiesiniam paraboliniam modeliui šakotose struktūrose su skirtingais srautų tvermės dėsniais išsišakojimo taškuose.
2. Atlikti neurono sužadinimo skaitinį modeliavimą, pritaikyti šiam uždaviniui ir ištirti lygiagrečiuosius algoritmus.
3. Atlikti parabolinio uždavinio su nelokalija integraline kraštine sąlyga skaitinę analizę, išnagrinėti skirtingus nelokalios sąlygos koeficientų reikšmių atvejus.
4. Atlikti netiesinio impulso relaksacijos puslaidininkyje skaitinį modeliavimą ir skaitinę analizę. Atlikti modelio identifikavimo eksperimentą.

Tyrimų metodika

Darbe atliktų tyrimų eigoje buvo taikomi diferencialinių lygčių dalinėmis išvestinėmis skaitiniai sprendimo metodai, jų konvergavimo ir stabilumo analizės metodai, taikomosios funkcinės analizės metodai, lygiagrečiųjų algoritmų konstravimo ir jų analizės metodai, globalios optimizacijos ir netiesinių matematinių modelių parametrų identifikuojamumo nustatymo metodai. Skaitinių eksperimentų programos parašytos C++ kalba, naudojant lygiagrečiąją biblioteką MPI, grafų dalijimo įrankį `Metis`; kai kurie skaičiavimo rezultatai lyginami su NEURON paketo pagalba gautais rezultatais.

Darbo mokslinis naujumas

Disertacijoje didelis dėmesys yra skiriamas tiesiniams modeliams grafuose, nes ląstelių sužadinimo modeliai pasižymi sąlyginiu tiesiškumu ir gali būti skaidomi į kelias tiesines sistemas. Daug mokslininkų nagrinėja skaitinius metodus sužadinimo modeliams, tačiau apsiribojama uždaviniais viename segmente. Disertacijoje ištirti du tvėrmės dėsniai išsišakojimo taškuose, jų skaitinei analizei atlikti pritaikyti būdai, naudojami tiriant antrojo ir trečiojo tipo kraštines sąlygas. Be tradiciškai taikomos šio tipo uždaviniams svorinės schemos ištirtos dvi prediktoriaus – korektorius tipo schemos, įrodytas šių schemų stabilumas ir sąlyginis konvergavimas. Parodyta, kad superpozicija grindžiamos neišreikštinės skaičiavimo schemos lygiagretinimo efektyvumas yra pakankamai aukštas, todėl ji gali būti sėkmingai naudojama lygiagrečiuose skaičiavimuose. Netiesiniam krūvininkų rekombinacijos apšviestame puslaidininkyje modeliui pasiūlyta ir išnagrinėta neiteracinė skaičiavimo schema, taikant kai kuriuos statistinius metodus išnagrinėtas modelio identifikavimo uždavinys.

Disertacijoje taip pat nagrinėjamas uždavinys su nelokaliąja integraline kraštine sąlyga. Atlikta sisteminga tokio tipo nelokalių sąlygų analizė visoje parametrų (a, b) plokštumoje. Pateikiama diskrečiosios neišreikštinės Eulerio schemos stabilumo analizė maksimumo normoje, pagerinti žinomi rezultatai. Integralinės kraštinės sąlygos atveju įrodytas uždavinio jautrumo integralinės sąlygos atžvilgiu įvertis, parodantis tik sąlyginį konvergavimą, ir pasiūlytas reguliarizuojantis sąryšis tarp diskrečiųjų žingsnių.

Darbo rezultatų praktinė reikšmė

Sudaryti ir realizuoti skaitiniai algoritmai, kurie leidžia modeliuoti reakcijos – difuzijos procesus šakotose struktūrose, tarp jų neurono sužadinimo procesą. Didelių struktūrų tyrimams realizuoti lygiagretieji algoritmai, pagrįsti duomenų lygiagretumo principu.

Realizuotas netiesinio sužadintų krūvininkų rekombinacijos modelio optimizavimo algoritmas. Pateikti parametrų identifikuojamumo tyrimo rezultatai rodo, kad ne visus modelio parametrus įmanoma nustatyti.

Ginamieji teiginiai

1. Diskrečių matematinių modelių grafuose tyrimui taikytini metodai, naudojami tiriant diskrečiuosius modelius su antrojo ir trečiojo tipo kraštinėmis sąlygomis.
2. Realizuotų lygiagrečiųjų algoritmų grafuose efektyvumas daugiausiai priklauso nuo duomenų paskirstymo kokybės ir branduolių konkurencijos dėl bendros atminties.
3. Vienmatės parabolinės lygties su nelokaliaja integraline sąlyga diskrečiosios schemos stabilumo ir konvergavimo sritis priklauso nuo nelokalsios sąlygos koeficientų ženklų.
4. Netiesinio krūvininkų rekombinacijos modelio diskretusis sprendinys atkartoja pagrindines diferencialinio sprendinio savybes. Modelio parametrų identifikuojamumas su naudojamais eksperimentiniais duomenimis yra ribotas.

Darbo rezultatų aprobavimas

Tyrimai atlikti Vilniaus Gedimino technikos universitete. Su disertacijos tema susiję rezultatai paskelbti 7 moksliniuose straipsniuose: 6 straipsniai publikuoti recenzuojamuose mokslo leidiniuose, iš jų 5 – leidiniuose įtrauktuose į *MII Web of Science* duomenų bazę. Disertacijos tema perskaityti 13 pranešimų Lietuvos ir kitų šalių konferencijose. Tyrimo rezultatai buvo pristatyti 4 Vilniaus Gedimino technikos universiteto Matematinio modeliavimo katedros seminaruose.

Disertacijos struktūra

Disertaciją sudaro įvadas, 5 skyriai, išvados ir literatūros sąrašas. 1-ajame skyriuje pateikta matematinių modelių nestandartinėse srityse arba su neklasikinėmis sąlygomis uždavinių apžvalga. 2-ajame skyriuje formuluojamas tiesinis parabolinis uždavinys grafuose, pateikiamos trys diskrečiosios baigtinių skirtumų schemos, schemų stabilumo ir konvergavimo analizė. 3-ajame skyriuje aprašomi lygiagretieji algoritmai paraboliniams uždaviniams grafuose, pateikiama šių algoritmų efektyvumo ir išplėčiamumo analizė ir skaičiavimo eksperimentų rezultatai. Taip pat šiame skyriuje aprašomas neuroninių ląstelių grupės sužadavimo modeliavimo eksperimentas. 4-ajame skyriuje nagrinėjamas vienmatis parabolinis uždavinys su nelokaliaja integraline sąlyga. Pateikiama neišreikštinė schema, schemos stabilumo ir konvergavimo analizė su skirtingomis nelokalsios sąlygos koeficientų reikšmėmis. Rezultatai lyginami su kitų mokslininkų paskelbtais rezultatais. 5-ajame skyriuje nagrinėjamas netiesinis sužadintų krūvininkų rekombinacijos uždavinys. Pateikiamas apriorinis sprendinio įvertis, neišreikštinė schema ir šios schemos analizė. Nagrinėjamos modelio parametrų nustatymo galimybės, o optimizavimo uždavinys sprendžiamas pasitelkus genetinį algoritmą. Pateikiami parametrų optimizavimo rezultatai.

Bendrosios išvados

Darbe buvo nagrinėjami paraboliniai uždaviniai šakotose struktūrose arba su integralinėmis kraštinėmis sąlygomis. Apibendrinsime pagrindinius rezultatus:

1. Sprendžiant reakcijos – difuzijos uždavinį šakotose struktūrose įrodytas neišreikštinės svorinės schemos besąlyginis stabilumas, kai svorinės schemos parametras $\theta \in [\frac{1}{2}, 1]$. Pavyko pagerinti gautus taikant maksimumo principą rezultatus ir įrodyti, kad konvergavimo greitis grafo viršūnėse yra toks pat, kaip ir vienmačio parabolinio uždavinio. Teoriniai rezultatai patvirtinti skaičiavimo eksperimento rezultatais.
2. Atlikta dviejų prediktoriaus – korektorius schemų, grindžiamų skirtingu skaičiavimo srities padalijimu, analizė. Taikant energetinius metodus įrodyta, kad abi prediktoriaus – korektorius schemos yra besąlygiškai stabilios, tačiau jų konvergavimas susijusioje normoje dėl prediktoriaus žingsnyje įneštos paklaidos yra sąlyginis. Naudojant prediktoriaus – korektorius ir Douglas schemų ekvivalentiškumą, gauti rezultatai palyginti su žinomu Douglas schemos konvergavimo įverčiu. Atlikto skaičiavimo eksperimento rezultatai patvirtina, kad prediktoriaus žingsnio netiktis yra $O(\tau^2/h)$.
3. Aprašytos lygiagrečiosios algoritmų versijos. Atlikta algoritmų efektyvumo ir išplėčiamumo analizė ir skaičiavimo eksperimentai rodo, kad prediktoriaus – korektorius schemų išplėčiamumas yra tiesinis, o neišreikštinės schemos blogiausiu atveju gali būti kvadratinis. Įrodyta, kad skaičiavimų efektyvumas daugiausiai priklauso nuo duomenų paskirstymo kokybės ir atminties magistralės riboto pralaidumo, kai yra naudojami 2 ar 4 branduoliai skaičiavimo mazge.
4. Atlikta parabolinio uždavinio su integrale kraštine sąlyga stabilumo analizė maksimumo normoje ir įrodyta, kad diskrečiosios schemos standumas ir stabilumo srities spindulys priklauso nuo nelokalių kraštinės sąlygos koeficientų ženklų. Pagerinti žinomi stabilumo rezultatai. Paprastos integralinės kraštinės sąlygos atveju įrodytas sąlyginis konvergavimas ir pasiūlytas reguliarizuojantis sąryšis tarp diskrečiųjų žingsnių.

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THE NUMERICAL ANALYSIS OF NONLINEAR MATHEMATICAL MODELS
ON GRAPHS

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

NETIESINIŲ MATEMATINIŲ MODELIŲ GRAFUOSE SKAITINĖ ANALIZĖ

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