The Alternating-Triangular Algorithm for the Analysis of Blow-Up and Quenching Phenomena in Nonlinear PDEs

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International Journal of Mathematical Algorithms, 2, 89-120, 2000

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IJMA. International Journal of Mathematical Algorithms

Short Title: Int. J. Math. Algorithms

Publisher: Gordon & Breach Science Publishers (Taylor & Francis Group), Reading; OPA (Overseas Publishers Association), Amsterdam

ISSN: 1027-9350

Melnik, R. V. N.

The alternating-triangular algorithm for the analysis of blow-up and quenching phenomena in nonlinear PDEs. (English) Zbl 0974.65083

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Reviewer: Song Jiang (Beijing)

MSC:

65M06 Finite difference methods for initial value and initial-boundary value problems involving PDEs
65N06 Finite difference methods for boundary value problems involving PDEs
35K65 Degenerate parabolic equations
80M20 Finite difference methods applied to problems in thermodynamics and heat transfer
35K57 Reaction-diffusion equations
80A20 Heat and mass transfer, heat flow (MSC2010)
82D37 Statistical mechanical studies of semiconductors
68W30 Symbolic computation and algebraic computation
65Y15 Packaged methods for numerical algorithms

Keywords:

alternating-triangular method; difference schemes; nonlinear parabolic and elliptic equations; 2-D initial boundary value problem; blow-up and quenching phenomena; numerical examples; reaction-diffusion problems; heat location; flame propagation; semiconductor devices; software package ALTPACK

Software:

ALTPACK

APPLICATION OF ALTPACK TO THE SOLUTION OF NONLINEAR PDEs

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Abstract

In this article the author applies the alternating-triangular method (ATM) to the solution of a number of 2D initial-boundary value problems that can be modelled by non-linear parabolic equations with a source term. Different types of non-linearities are considered and the procedure of finding approximate solutions is explained. The main features of the ALTPACK package are outlined and the results of computational experiments are presented.

Key words: non-linear parabolic equations with source terms, alternating-triangular method.

1 Introduction.

The application of mathematical models based on linear and nonlinear elliptic and parabolic equations is extremely wide [2, 6, 10, 15, 23, 9, 16]. It includes such areas as heat conduction, diffusion, electron and ion thermoconductivity, combustion and porous media modelling, chemical kinetics, semiconductor device modelling, biophysics etc. Such models differ from each other only by types of dependencies of coefficients and source terms. From the point of view of constructive investigations it is exactly such types that define the "fingerprint" of a specific model. In some cases such "fingerprints" may be treated using quite general techniques, while in other they require individual approaches [21].

For a start let us consider the linear equation of thermoconductivity. It is known that the fundamental solution of the operator

$$\mathcal{L}(\Phi) = \frac{\partial \Phi}{\partial t} - c^2 \Delta \Phi, \tag{1.1}$$

in the space-time region $R^n \times R_+$, i.e. the solution of the equation

$$\mathcal{L}(\Phi) \equiv \frac{\partial \Phi}{\partial t} - c^2 \Delta \Phi = \delta(\mathbf{x}, t), \tag{1.2}$$

can be expressed as

$$\Phi(\mathbf{x}, t) = \frac{H(t)}{(2c\sqrt{\pi t})^n} e^{-\frac{|\mathbf{x}|^2}{4c^2 t}}, \tag{1.3}$$

where $H(t)$ is the Heviside function, $\mathbf{x} = (x_1, ..., x_n)$ and c is the thermoconductivity coefficient (see, for example, [23]). Theoretically the solution (1.3) gives the distribution of temperature from the point instant source $\delta(\mathbf{x})\delta(t)$. However since $\Phi(\mathbf{x}, t) > 0 \; \forall \; t > 0, \mathbf{x} \in R^n$ one observes that such a solution might be an adequate approximation of the heat transfer process only under certain constraints (such as large values of $\mathbf{x}$ and small values of t). Since such constraints may not conform to many applied problems in a number of situations it is reasonable either

- to use a nonlinear thermoconductivity equation, or
- to apply integro-differential transport equation

in order to describe heat processes more precisely. In the later case such an integro-differential equation may incorporate non-locality and memory effects, and gives a parabolic equation only in the limit of small deviations from the equilibrium state [11]. It is also possible to consider a hyperbolic heat equation [1, 17] and/or to take into account the influence of non-thermal physical fields [13].

In its essence all of the above options can be cast in an equation of the following type

$$u_t = A(u, f), \tag{1.4}$$

where $A(u, f)$ is a differential or integro-differential operator, and the functional f represents source-related terms. In all applied problems the definition of such a functional f is the subject of an approximation. For a specific choice f there may exist a stationary solution u^* such that

$$A(u^*, f) = 0, \tag{1.5}$$

and in this case one may expect that

$$u(\cdot, t) \to u^* \;\; \text{when} \;\; t \to \infty. \tag{1.6}$$

However, in the general case there are such approximations f that certain measures of the $u(\cdot, t)$ tends to infinity when time approaches a finite critical value. In the latter case it is reasonable to seek such an approximate solution(s) of the equation (1.4) that will be a stationary solution y^* of another equation

$$y_t = \tilde{A}(y, \tilde{f}), \tag{1.7}$$

i.e. such that $u \approx y^*$, where $\tilde{A}(y^*, \tilde{f}) = 0$. For example, there exist a large class of problems (1.4) for which the equation (1.7) is the Hamilton-Jacobi-Bellman-type equation [3, 5].

The equation (1.7) may be seen as an asymptotic approximation of (1.4) with respect to a certain small parameter ϵ which is included into the original equation implicitly (or in some cases explicitly) by the nonlinearities of sources and/or equation coefficients. Although the asymptotic behaviour of (1.4) may be controlled by stationary solutions of (1.7), the efficiency of such a control is essentially dependent on ϵ. In other words, ϵ may be small, but it is always positive, and as a result, y may appear to be a very rough approximation to u for fairly large intervals of time.

Ideally, investigations of parabolic models have to blend asymptotic and numerical techniques for their solution. In many cases asymptotic approximations may give an important qualitative perception of the solution and provide certain guidelines for the obtaining of quantitative picture by a numerical method. The major difficulties with asymptotic approaches lie with an approximate nature of the functional f in the model (1.4). Considering real physical processes in non-linear dissipative media one has to specify the law of energy loss in order to make the model relevant to the real-world applications. In many cases such specifications may be incorporated approximately through the boundary conditions of the problem (for example,

in the combustion theory we often have to take into account the loss of heat on the boundaries of the flame region). Conceptually, approximations (incorporated into the model through nonlinearities, initial and boundary conditions) lead to a continuum set of possibilities in the simulation of the evolution of dissipative processes. In each specific case such approximations may give rise to discrete space-time scales [21], which can be often grasped numerically with a required accuracy [4]. Therefore, in order to reveal the structure of dissipative processes numerical methods will remain a major and the most natural tool in investigations of the evolutions of such processes in non-homogeneous dissipative media.

In this paper we apply an effective numerical method to a number of nonlinear problems that recently attracted a lot of attention of researchers [21, 5, 8]. In a vast majority of cases such attention was devoted to the Cauchy problem for non-linear parabolic equations. Moreover, the application of asymptotic techniques to the investigation of space-time architecture of dissipative structures were often limited to the one dimensional case. In this paper we consider initial-boundary value problems in the two dimensional case. Main examples concern model problems that arise from complex mathematical models in semiconductor device modelling, porous media, combustion theory, reaction-diffusion applications and other applications [16, 9, 14, 10, 6, 2, 15].

The remaining part of the paper is organised as follows.

• In Section 2 we introduce notation that is used throughout the paper.

• Section 3 is devoted to the formulation of the mathematical model that is being investigated numerically.

• Section 4 describes with the main steps of the integro-interpolational approach applied for the construction of difference schemes for the problem.

• Section 5 deals with the alternating-triangular method applied to the solution of discrete problems that arise at each time-layer.

• Section 6 is devoted to the choice of accelerating parameters for the ATM.

• Algorithmic aspects of the alternating-triangular method are discussed in Section 7.

• In Section 8 we present results of computational experiments on the application of the described procedure.

2 Notation

The following notations are used throughout the article.

- $G = \{x = (x_1, x_2) : \ 0 \le x_i \le L_i, \ i = 1, 2 \ T \ \}$ denotes the spatial region of interest;
- $\bar{G} = G \cup \Gamma$ is the closed region, where Γ denotes its boundaries;
- $\bar{T} = \{t : \ 0 \le t \le T_f\}$ denotes the temporal interval of consideration with the final time denoted by T_f;
- $\hat{\omega}_h = \hat{\omega}_1 \times \hat{\omega}_2$, denotes a nonuniform grid that covers the region $\bar{G}$;
- $\hat{\omega}_1 = \{x_{1,i_1} \in [0, L_1] : \ x_{1,i_1} = x_{1,i_1-1} + h^-_{1,i_1}, \ i_1 = 0, ..., N_1, \ x_{1,0} = 0, \ x_{1,N_1} = L_1\}$;
- $\hat{\omega}_2 = \{x_{2,i_2} \in [0, L_2] : \ x_{2,i_2} = x_{2,i_2-1} + h^-_{2,i_2}, \ i_2 = 0, ..., N_2, \ x_{2,0} = 0, \ x_{2,N_2} = L_2\}$;
- $\hat{\omega}_{h\tau} = \bar{\omega}_\tau \times \hat{\omega}_h$, where $\bar{\omega}_\tau = \{t_k = k\tau, \ k = 0, ..., L, \ L\tau = T_f\}$;
- ω_i denotes the set of all inner points of the grid $\hat{\omega}_i$, i=1,2, and $\omega_h = \omega_1 \times \omega_2$;
- γ_i - is the set of all boundary points in $x_j \in [0, L_j]$ when $x_i = 0$ and $x_i = L_i, \ i = 1, 2, \ j = 3 - i$ (hence the boundary of the grid $\hat{\omega}_h$ is defined by $\gamma = \gamma_1 \cup \gamma_2$ and $\hat{\omega}_h = \omega_h \cup \gamma$);

- $\omega_i(x_j)$ are points of the grid ω_h for fixed x_j, and $\hat{\omega}_i(x_j)$ denotes the set of points of the grid $\hat{\omega}_h$ for fixed x_j;
- $\omega_i^+(x_j)$ - is the set of points of the grid $\omega_i(x_j)$ plus the node $x_i = L_i$;
- $\omega_i^-(x_j)$ - the set of points of the grid $\omega_i(x_j)$ plus the node $x_i = 0$;
- $h^+_{1,i_1} = h^-_{1,i_1+1}, \;\; h^+_{2,i_2} = h^-_{2,i_2+1}$;
- $\hbar_{1,i_1} = 0.5(h^-_{1,i_1} + h^+_{1,i_1}), \;\; \hbar_{2,i_2} = 0.5(h^-_{2,i_2} + h^+_{2,i_2})$;
- $\hbar_{i,0} = 0.5h^+_{i,0}, \;\; \hbar_{i,N_i} = 0.5h^-_{i,N_i}, \; i = 1, 2$;
- $x_{1,i_1 \pm 0.5} = x_{1,i_1} \pm 0.5h^{\pm}_{1,i_1}, \; x_{2,i_2 \pm 0.5} = x_{2,i_2} \pm 0.5h^{\pm}_{2,i_2}$.

Let further $y = y(x_1, x_2, t) \equiv y(i_1, i_2, k)$ be a function of discrete arguments $\mathbf{x} = (x_1, x_2)$ and t defined on a non-uniform grid $\hat{\omega}_{h\tau}$. Then we use the standard notation for difference derivatives of y [19, 20, 14, 22]. For example for a function of $\tilde{y}$ of one one variable defined on $\hat{\omega}_1$

- the backward difference derivative is

$$\tilde{y}_{\bar{x}_1} = \frac{\tilde{y}_{i_1} - \tilde{y}_{i_1-1}}{h_{1,i_1}},$$

- the forward difference derivative is

$$\tilde{y}_{x_1} = \frac{\tilde{y}_{i_1+1} - \tilde{y}_{i_1}}{h_{1,i_1+1}},$$

- and the second ("central") difference derivative is

$$\tilde{y}_{\bar{x}_1\hat{x}_1} = \frac{1}{\hbar_{i_1}} \left[\frac{\tilde{y}_{i_1+1} - \tilde{y}_{i_1}}{h_{i_1+1}} - \frac{\tilde{y}_{i_1} - \tilde{y}_{i_1-1}}{h_{i_1}} \right].$$

By $\mathcal{H}$ we denote the space of grid functions that are defined on $\hat{\omega}_h$ with the scalar product and the norm defined as follows

$$(u, v) = \sum_{\hat{\omega}} u(x)v(x)\hbar_1\hbar_2, \;\; \|u\| = \sqrt{(u, u)}, \qquad \forall \; u(x), v(x) \in \mathcal{H}.$$

In an analogous way we define the scalar products on $\omega_i^+(x_j)$, $\hat{\omega}_i(x_j)$ and $\omega_i^+ \times \hat{\omega}_j$

$$(u, v)_{\omega_i^+(x_j)} = \sum_{\omega^+(x_j)} u(x)v(x)h_i^-, \;\; (u, v)_{\hat{\omega}_i(x_j)} = \sum_{\hat{\omega}_i(x_j)} u(x)v(x)\hbar_i,$$

$$\text{and} \;\; (u, v)_i = \sum_{\omega_i^+ \times \hat{\omega}_j} u(x)v(x)\hbar_i^-\hbar_j, \qquad i = 1, 2, \;\; j = 3 - i.$$

Other notation used in this paper are standard in theory of difference schemes [22, 19, 14, 20].

3 Mathematical model

In the space-time region $\bar{Q}_T = \bar{G} \times \bar{T}$ we consider a general type of nonlinear partial differential equation

$$a^0(\mathbf{x}, t, u)\frac{\partial u}{\partial t} = \sum_{i=1}^{2} \frac{\partial}{\partial x_i} \left[k_i(\mathbf{x}, t, u)\frac{\partial u}{\partial x_i} \right] - q^0(\mathbf{x}, t, u))u + f^0(\mathbf{x}, t, u), \tag{3.1}$$

where $\mathbf{x} = (x_1, x_2)$, and a^0, q^0, f^0, k_i, $i = 1, 2$ are given functions of $\mathbf{x}, t$ and u. Equation (3.1) is supplemented by the initial

$$u(x_1, x_2, 0) = u_0(x_1, x_2) \tag{3.2}$$

and boundary conditions

$$\lambda_i^{(1)} \frac{\partial u}{\partial x_i} = \kappa_i^{(1)}(x_j, t, u)u - g_i^{(1)}(x_j, t, u), \qquad x_i = 0, \tag{3.3}$$

$$-\lambda_i^{(2)} \frac{\partial u}{\partial x_i} = \kappa_i^{(2)}(x_j, t, u)u - g_i^{(2)}(x_j, t, u), \qquad x_i = L_i,\ i = 1, 2,\ j = 3 - i. \tag{3.4}$$

In (3.3) and (3.4) values of $\lambda_i^{(1)}$ and $\lambda_i^{(2)}$ are equal 1 if on the corresponding boundaries of the spatial region G we are given the Neumann or the 3rd kind boundary conditions. They equal zero for the Dirichlet boundary conditions.

Mathematical model (3.1)–(3.4) describes a wide range of phenomena from physics, chemistry, biology and economics. For example, many reaction-diffusion problems, models for heat localisation and flame propagation may be cast in the form (3.1)–(3.4). Solutions of such non-linear evolutionary problems even in the simplest one-dimensional case may form finite time singularities, exhibit blow-up or extinction behaviour. Investigation of such a behaviour in dissipative media is the first step in the simulation of evolution of non-equilibrium open thermodynamical systems [21].

In such a general formulation as (3.1)–(3.4) theoretical issues of existence and uniqueness of the solution lie outside of the scope of this paper. The reader has to consult [21, 5, 8] and references therein in order to get more details on existence/nonexistence of arising problems. For the purposes of this paper we limit ourselves to the situation when the coefficients in (3.1)–(3.4) satisfy the following conditions

$$\kappa_i^1(x_j, t, u) \geq 0,\ \kappa_i^2(x_j, t, u) \geq 0,\ 0 < c' \leq k_i(\mathbf{x}, t, u) \leq c'', q^0(\mathbf{x}, t, u) \geq 0. \tag{3.5}$$

The condition (3.5) includes the possibility of fast changing coefficients. Problems with such coefficients arise naturally in many practical situations [10, 6, 9, 16]. Such problems, rarely treatable analytically, cause serious mathematical difficulties and require the application of effective numerical methods. In what follows we describe mathematics of the software package ALTPACK, designed for the solution of a general class of problems (3.1)–(3.4), and present the results of computational experiments.

4 Discrete Conservation Laws and Integro-Interpolational Approach

We cover the region $\bar{Q}_T$ with a non-uniform grid $\hat{\omega}_{h\tau}$ and consider an elementary space-time cell, Δ_{st}, defined as $\Delta_{st} = \Delta_s \times \Delta_t$, where $\Delta_t = \{t_k \leq t \leq t_k + \tau\}$ and

$$\Delta_s = \{(x_1, x_2) :\ x_{1,i_1-0.5} \leq x_1 \leq x_{1,i_1+0.5},\ x_{2,i_2-0.5} \leq x_2 \leq x_{2,i_2+0.5}\ \}.$$

Let $\mathcal{F}^{(i)}(\mathbf{x}, t, u)$ be the flux in the direction of x_i, i.e.

$$\mathcal{F}^{(i)}(\mathbf{x}, t, u) = k_i(\mathbf{x}, t, u) \frac{\partial u}{\partial x_i}. \tag{4.1}$$

The construction of difference schemes for the solution of problem (3.1)–(3.4) is conducted by the integro-interpolational method [19, 20]. Below we explain the main ideas of such a construction.

Let us integrate differential equation (3.1) over the cell Δ_{st}. We obtain the following balance equation

$$\int_{t_k}^{t_k+\tau}\left\{\int_{x_2,i_2-0.5}^{x_2,i_2+0.5}\left[\mathcal{F}^{(1)}_{i_1+0.5}(x_2)-\mathcal{F}^{(1)}_{i_1-0.5}(x_2)\right]dx_2dt+\right.$$
$$\left.\int_{x_1,i_1-0.5}^{x_1,i_1+0.5}\left[\mathcal{F}^{(2)}_{i_2+0.5}(x_1)-\mathcal{F}^{(2)}_{i_2-0.5}(x_1)\right]dx_1dt\right\}-\int_{\Delta_{st}}q^0(\mathbf{x},t,u)ud\mathbf{x}dt=$$
$$\int_{\Delta_{st}}a^0(\mathbf{x},t,u)\frac{\partial u}{\partial t}d\mathbf{x}dt-\int_{\Delta_{st}}f^0(\mathbf{x},t,u)d\mathbf{x}dt, \tag{4.2}$$

where $d\mathbf{x}\equiv dx_1dx_2$ and

$$\mathcal{F}^{(1)}_{i_1\pm0.5}(x_2)=\mathcal{F}^{(1)}(x_{1,i_1\pm0.5},x_2),\quad \mathcal{F}^{(2)}_{i_2\pm0.5}(x_1)=\mathcal{F}^{(2)}(x_1,x_{i_2\pm0.5}).$$

First we divide identity (4.1) by $k_i(\mathbf{x},t,u), i=1,2$ and integrate the result over the intervals $[x_{1,i_1},x_{1,i_{1,i_1+1}}]$ and $[x_{2,i_2},x_{2,i_{2,i_2+1}}]$ respectively. We get

$$u(x_{1,i_1+1},x_2,t)-u(x_{1,i_1},x_2,t)=\int_{x_{1,i_1}}^{x_{1,i_1+1}}\frac{\mathcal{F}^{(1)}(\mathbf{x},t,u)}{k_1(\mathbf{x},t,u)}dx_1, \tag{4.3}$$

$$u(x_1,x_{2,i_2+1},t)-u(x_1,x_{2,i_2},t)=\int_{x_{2,i_2}}^{x_{2,i_2+1}}\frac{\mathcal{F}^{(2)}(\mathbf{x},t,u)}{k_2(\mathbf{x},t,u)}dx_2. \tag{4.4}$$

Then we use the following interpolation formulas

$$\mathcal{F}^{(1)}(\mathbf{x},t,u)\approx\mathcal{F}^{(1)}_{i_1+0.5}(x_2,t,u),\quad \text{where } x_1\in[x_{1,i_1},x_{1,i_1+1}] \tag{4.5}$$

and

$$\mathcal{F}^{(2)}(\mathbf{x},t,u)\approx\mathcal{F}^{(2)}_{i_2+0.5}(x_1,t,u),\quad \text{where } x_2\in[x_{2,i_2},x_{2,i_2+1}]. \tag{4.6}$$

Substituting (4.5) and (4.6) into (4.3), (4.4) respectively, we come to the following approximate equalities

$$u(x_{1,i_1+1},x_2,t)-u(x_{1,i_1},x_2,t)\approx\mathcal{F}^{(1)}_{i_1+0.5}(x_2,t,u)\int_{x_{1,i_1}}^{x_{1,i_1+1}}\frac{dx_1}{k_1(\mathbf{x},t,u)}, \tag{4.7}$$

$$u(x_1,x_{2,i_2+1},t)-u(x_1,x_{2,i_2},t)\approx\mathcal{F}^{(2)}_{i_2+0.5}(x_1,t,u)\int_{x_{2,i_2}}^{x_{2,i_2+1}}\frac{dx_2}{k_2(\mathbf{x},t,u)}. \tag{4.8}$$

The next step of the procedure is to express the values of $\mathcal{F}^{(1)}_{i_1\pm0.5}(x_2,t,u)$ and $\mathcal{F}^{(2)}_{i_2\pm0.5}(x_1,t,u)$ through the solution of the problem and known functions. It can be easily done from (4.7), (4.8). Indeed, dividing (4.7) and by h^+_{1,i_1} and then by h^-_{1,i_1} we have

$$\mathcal{F}^{(1)}_{i_1+0.5}(x_2,t,u)\approx u_{x_1,i_1}\left[\frac{1}{h^+_{1,i_1}}\int_{x_1,i_1}^{x_1,i_1+1}\frac{dx_1}{k_1(\mathbf{x},t,u)}\right]^{-1}, \tag{4.9}$$

$$\mathcal{F}^{(1)}_{i_1-0.5}(x_2,t,u)\approx u_{\bar{x}_1,i_1}\left[\frac{1}{h^-_{1,i_1}}\int_{x_1,i_1-1}^{x_1,i_1}\frac{dx_1}{k_1(\mathbf{x},t,u)}\right]^{-1} \tag{4.10}$$

Analogous expressions can be obtained for $\mathcal{F}^{(2)}_{i_2\pm0.5}$ from (4.8).

The integro-difference scheme for the solution of the problem (3.1)–(3.4) follows after substitution (4.9), (4.10) (and analogous expressions for $\mathcal{F}^{(2)}_{i_2\pm0.5}$) into (4.2). The application of

interpolational formulas for the remaining functions in the integrals in (4.2) leads to a fully discrete approximation of the model (3.1)–(3.4). Such discrete approximations tend to preserve on the grid conservative properties of the process expressed by (4.2), and are usually referred to as conservative difference schemes [19, 22]. For example, in the linear case of elliptic equations we get [20]

$$\sum_{i=1}^{2}(\mathcal{K}_i y_{\bar{x}_i})_{\hat{x}_i} - qy = -f, \quad x \in \omega_h, \tag{4.11}$$

i.e. for each inner node (i_1, i_2) we have the following equation

$$\frac{\mathcal{K}_1^+ y_{x_1} - \mathcal{K}_1 y_{\bar{x}_1}}{\hbar_{1,i_1}} + \frac{\mathcal{K}_2^+ y_{x_2} - \mathcal{K}_2 y_{\bar{x}_2}}{\hbar_{2,i_2}} - qy = -f, \tag{4.12}$$

where $y \equiv y(i_1, i_2)$ and the coefficients and the RHS in (4.12) are defined as follows

$$q \equiv q(i_1, i_2) = \frac{1}{\hbar_{1,i_1}\hbar_{2,i_2}} \int_{\Delta s} q^0(\mathbf{x}) d\mathbf{x}, \quad f \equiv f(i_1, i_2) = \frac{1}{\hbar_{1,i_1}\hbar_{2,i_2}} \int_{\Delta_s} f^0(\mathbf{x}) d\mathbf{x}, \tag{4.13}$$

$$\mathcal{K}_1 \equiv \mathcal{K}_1(i_1, i_2) = \frac{1}{\hbar_{2,i_2}} \int_{x_2,i_2-0.5}^{x_2,i_2+0.5} \left[\frac{1}{h^-_{1,i_1}} \int_{x_1,i_1-1}^{x_1,i_1} \frac{dx_1}{k_1(\mathbf{x})} \right]^{-1} dx_2 \tag{4.14}$$

(with an analogous formula for $\mathcal{K}_2$), $\mathcal{K}_1^+ \equiv \mathcal{K}_1^+(i_1, i_2) = \mathcal{K}_1(i_1 + 1, i_2)$, $\mathcal{K}_2^+ \equiv \mathcal{K}_2^+(i_1, i_2) = \mathcal{K}_2(i_1, i_2 + 1)$.

When the coefficients in (3.1)–(3.4) are smooth functions, then instead of (4.13), (4.14) we may use simplified expressions for the computation of coefficients and the RHS of (4.11) at each inner node (i_1, i_2). For example, $q = q^0(x_{1,i_1}, x_{2,i_2})$, $f = f^0(x_{1,i_1}, x_{2,i_2})$, $\mathcal{K}_1 = k_1(x_{1,i_1-0.5}, x_{2,i_2})$, $\mathcal{K}_2 = k_2(x_{1,i_1}, x_{2,i_2-0.5})$.

Let us consider the approximation of boundary conditions of problem (3.1)–(3.4) when $x_i = L_i$, $i = 1, 2$. We apply a 3-step procedure that consists of

- integrating the original differential equation over the cells

$$\Delta_s^{(1)} = \{(x_1, x_2) : \ L_1 - 0.5h^-_{1,N_1} \le x_1 \le L_1, \ x_{2,i_2-0.5} \le x_2 \le x_{2,i_2+0.5}\},$$
$$\Delta_s^{(2)} = \{(x_1, x_2) : \ L_2 - 0.5h^-_{2,N_2} \le x_2 \le L_2, \ x_{1,i_1-0.5} \le x_1 \le x_{1,i_1+0.5} \ \},$$

- using approximate formulas (4.9), (4.10) (and analogous expressions for $\mathcal{F}^{(2)}_{i_2\pm0.5}$), and
- computing values of $\mathcal{F}^{(1)}_{N_1}(x_2)$, $\mathcal{F}^{(2)}_{N_2}(x_1)$, from boundary condition (3.4) for $x_i = L_i = x_{i,N_i}$, $i = 1, 2$.

As a result of such a procedure we get

$$\frac{1}{\hbar_i}\left(g_i^{(2)} - \kappa_i^{(2)} y - \mathcal{K}_i y_{\bar{x}_i}\right) + \left(\mathcal{K}_j y_{\bar{x}_j}\right)_{\hat{x}_j} - qy = -f, \ x \in \hat{\omega}_j(L_i), \ i = 1, 2, \ j = 3 - i, \tag{4.15}$$

where for the grid prototypes of functions $\kappa_i^{(2)}$ and $g_i^{(2)}$ in (3.4) we used the same notation. In a similar way we construct the approximation of the boundary condition (3.3) for $x_i = 0$:

$$\frac{1}{\hbar_i}\left(\mathcal{K}_i^+ y_{x_i} - \kappa_i^{(1)} y + g_i^{(1)}\right) + \left(\mathcal{K}_j y_{\bar{x}_j}\right)_{\hat{x}_j} - qy = -f, \ x \in \hat{\omega}_j(0). \tag{4.16}$$

where, as above, $\kappa_i^{(1)}$ and $g_i^{(1)}$ are discrete prototypes of functions $\kappa_i^{(1)}$ and $g_i^{(1)}$ from (3.3).

5 Alternating-Triangular Method with Ordered Chebyshev Set of Iterative Parameters

The discrete scheme constructed in the previous section can be written in the following generic form

$$\Lambda y \equiv \sum_{i=1}^{2} \Lambda_i y = -\varphi, \quad x \in \hat{\omega}_h, \tag{5.1}$$

where $\varphi = f + \varphi_1 + \varphi_2, \quad x \in \hat{\omega}_h$, and for $i = 1, 2$

$$\Lambda_i y = \begin{cases} \frac{2}{h_i^+}\mathcal{K}_i^+ y_{x_i} - \left(\frac{2}{h_i^+}\kappa_i^{(1)} + \frac{1}{2}q\right) y, & x_i = 0, \\ (\mathcal{K}_i y_{\bar{x}_i})_{\hat{x}_i} - \frac{1}{2}qy, & x_i \neq 0, L_i, \\ -\frac{2}{h_i^-}\mathcal{K}_i y_{\bar{x}_i} - \left(\frac{2}{h_i^-}\kappa_i^{(2)} + \frac{1}{2}q\right) y, & x_i = L_i, \quad x_j \in \hat{\omega}_j, \end{cases} \qquad \varphi_i = \begin{cases} \frac{2}{h_i^+}g_i^{(1)}, & x_i = 0, \\ 0, & x_i \neq 0, L_i, \\ \frac{2}{h_i^-}g_i^{(2)}, & x_i = L_i, \quad x_j \in \hat{\omega}_j. \end{cases}$$

A special case of our scheme is a rectangular uniform grid in (x_1, x_2) when $h_\alpha^- = h_\alpha^+ = h_\alpha$. In such a case the difference scheme (5.1) with coefficients computed by the formulas (4.13), (4.14) will approximate the problem with error $O(|h|^2)$, where $|h|^2 = h_1^2 + h_2^2$ [20].

The scheme (5.1) can be applied for the solution of linear elliptic equations. In the general case of (3.1)–(3.4) on each time layer we can represent the difference scheme constructed by the described methodology as

$$Ay = \varphi, \tag{5.2}$$

with an operator $A : \mathcal{H} \to \mathcal{H}$ acting in the Hilbert space $\mathcal{H}$. More precisely, for the general non-stationary case we have to solve (5.2) on each time layer with an operator A which is a modified version of the operator Λ used in (5.1). In its essence we pass from nonstationary solution(s) of (3.1)–(3.4) to a sequence of stationary solutions for a family of problems that can be formally expressed in the form (1.7). The form of operator $\tilde{A}$ and the function $\tilde{f}$ in (1.7) are now well defined for each element of such a sequence of stationary solutions.

For the solution of problem (5.2) we apply an implicit two-layer scheme of the following general form

$$B(y_{k+1} - y_k)/\tau_{k+1} + Ay_k = \varphi, \ k = 0, 1, 2, ..., \ \forall y_0 \in \mathcal{H}. \tag{5.3}$$

Majority of known iterative procedures (such as the Zeidel method or upper-relaxation algorithm) are just partial cases of the scheme (5.3). They immediately follow from (5.3) if an appropriate choice of sequence $\{\tau_{k+1}\}$ is made and operator B is constructed. In order to make the method effective one has to choose the set of $\{\tau_{k+1}\}$ in some optimal way whereas B has to be constructed as a product of easily invertible operators. In this paper we use the alternating-triangular method with the optimal Chebyshev choice of parameters [7, 20]. We choose the operator B in the form

$$B = (D + \omega_0 A_1)D^{-1}(D + \omega_0 A_2), \ \omega_0 > 0, \tag{5.4}$$

where

$$Dy = d(\mathbf{x})y, \ d(\mathbf{x}) > 0, \ \mathbf{x} \in \hat{\omega}_h, \ A = A_1 + A_2, \ A_1^* = A_2. \tag{5.5}$$

We assume that inequalities

$$\delta D \leq A, \ A_1 D^{-1} A_2 \leq \frac{\Delta}{4} A, \ \delta > 0, \ \Delta > 0 \tag{5.6}$$

are satisfied with certain constants δ and Δ. Then we define parameters τ_{k+1} and ω_0 in the following way

$$\omega_0 = 2\sqrt{\delta\Delta},\ \tau_k = \frac{\tau_0}{1+\rho_0\sigma_k^*}, \tag{5.7}$$

where

$$\tau_0 = \frac{2}{\gamma_1^*+\gamma_2^*},\ \gamma_1^* = \frac{\delta}{2(1+\sqrt{\eta})},\ \gamma_2^* = \frac{\delta}{4\sqrt{\eta}},\ \rho = \frac{1-\psi}{1+\psi},\ \psi = \frac{\gamma_1^*}{\gamma_2^*},\ \eta = \frac{\delta}{\Delta},$$

and $\sigma_k \in \Sigma_{n_0}^*,\ k = 1, ..., n_0$. The set

$$\Sigma_{n_0}^* = \left\{ \cos\frac{2i-1}{2n_0}\pi,\ 1 \le i \le n_0 \right\} \tag{5.8}$$

is a specially ordered set of the roots of Chebyshev polynomial degree n_0. For more details on the ordering procedure the reader may consult [19, 20].

Remark 5.1 *In order to keep a trade-off between the accuracy of the approximate solution of (3.1)-(3.4) and the computational complexity of the procedure, we use an estimate of the number of ATM iterations for the given accuracy. If the error of the ATM has to be decreased by the factor of ε it is sufficient to perform n_0 iterations, where*

$$n_0 \ge \frac{\ln(2/\epsilon)}{2\sqrt{2}\sqrt[4]{\eta}}.$$

In the next section we define the operators $A_i,\ i = 1, 2$ in the case of linear elliptic problems and show how the choice of δ and Δ can be made in the general case.

6 The Choice of Accelerating Parameters δ and Δ

In order to compute the iterative parameter ω_0 in (5.7) we follow the procedure described in [19, 20] and proved to be effective in a number of applications (see, for example, [10, 6]).

Using the first Green's formula [19] for the special case of (5.1) where $\lambda_i^{(1)} = \lambda_i^{(2)} = 1$, we have

$$(Ay, y) = \sum_{i=1}^{2} \left((\mathcal{K}_i y_{\bar{x}_i}^2, 1)_i + (\kappa_i^{(1)} y^2, 1)_{\hat{\omega}_j(0)} + (\kappa_i^{(2)} y^2, 1)_{\hat{\omega}_j(L_i)} \right) + (qy^2, 1),\ j = 3-i. \tag{6.1}$$

We define the operator A in (5.2) as the sum of operators A_1 and A_2, where

$$A_i = A_i^{(1)} + A_i^{(2)},\ \ i = 1, 2,$$

and

$$A_1^{(i)} y = \begin{cases} \frac{1}{2}\left[\frac{2}{h_i^+}\left(\frac{\mathcal{K}_i^+}{h_i^+} + \kappa_i^{(1)}\right) + \frac{1}{2}q\right] y, & x_i = 0, \\ \frac{\mathcal{K}_i}{\hbar_i} y_{\bar{x}_i} + \frac{1}{2}\left[\frac{1}{\hbar_i}\left(\frac{\mathcal{K}_i^+}{h_i^+} - \frac{\mathcal{K}_i}{h_i^-}\right) + \frac{1}{2}q\right] y, & x_i \ne 0, L_i, \\ \frac{2}{h_i^-}\mathcal{K}_i y_{\bar{x}_i} + \frac{1}{2}\left[\frac{2}{h_i^-}\left(\kappa_i^{(2)} - \frac{\mathcal{K}_i}{h_i^-}\right) + \frac{1}{2}q\right] y, & x_i = L_i,\ \ x_j \in \hat{\omega}_j \end{cases}$$

$$A_2^{(i)} y = \begin{cases} -\frac{2}{h_i^+}\mathcal{K}_i y_{x_i} + \frac{1}{2}\left[\frac{2}{h_i^+}\left(\kappa_i^{(1)} - \frac{\mathcal{K}_i^+}{h_i^+}\right) + \frac{1}{2}q\right] y, & x_i = 0, \\ -\frac{\mathcal{K}_i^+}{\hbar_i} y_{x_i} + \frac{1}{2}\left[\frac{1}{\hbar_i}\left(\frac{\mathcal{K}_i}{h_i^-} - \frac{\mathcal{K}_i^+}{h_i^+}\right) + \frac{1}{2}q\right] y, & x_i \ne 0, L_i, \\ \frac{1}{2}\left[\frac{2}{h_i^-}\left(\frac{\mathcal{K}_i}{h_i^-} + \kappa_i^{(2)}\right) + \frac{1}{2}q\right] y, & x_i = L_i, x_j \in \hat{\omega}_j. \end{cases}$$

It can be verified that $A_1^* = A_2$ and $A = A_1 + A_2$. Therefore

$$(A_1 D^{-1} A_2 y, y) = (D^{-1} A_2 y, A_2 y) = (D^{-1}(A_2 y)^2, 1) = \left(D^{-1} \left[\sum_{i=1}^{2} A_2^{(i)} y \right]^2, 1 \right).$$

Assuming that the function $d(\mathbf{x})$ (see (5.5)) has the following form

$$d(\mathbf{x}) = d_1(\mathbf{x}) + d_2(\mathbf{x}), \ \mathbf{x} \in \hat{\omega}_h,$$

where

$$d_i(\mathbf{x}) = \begin{cases} \left(2\mathcal{K}_i^+ + h_i^+ \Omega_i \left| \kappa_i^{(1)} - \frac{\mathcal{K}_i^+}{h_i^+} + \frac{h_i^+}{4} q \right| \right) \frac{\Theta_i}{(h_i^+)^2}, & x_i = 0, \\ \left(\mathcal{K}_i^+ + \frac{h_i^+ \Omega_i}{2} \left| \frac{\mathcal{K}_i}{h_i^-} - \frac{\mathcal{K}_i^+}{h_i^+} + \frac{\hbar_i}{2} q \right| \right) \frac{\Theta_i}{\hbar_i h_i^+}, & x_i \neq 0, L_i, \\ \left| \kappa_i^{(2)} + \frac{\mathcal{K}_i}{h_i^-} + \frac{h_i^-}{4} q \right| \frac{\Omega_i \Theta_i}{h_i^-}, & x_i = L_i, \ \ x_j \in \hat{\omega}_j, \end{cases}$$

and $\Omega_i = \Omega_i(x_j)$, $\Theta_i = \Theta_i(x_j)$ are certain grid functions that are positive on $\hat{\omega}_h$ (precise definitions are given below). Then applying ϵ- inequality [19, 14] it is straightforward to get

$$(A_1 D^{-1} A_2 y, y) \leq \sum_{i=1}^{2} \left[\left(\frac{\mathcal{K}_i}{\Theta_i} y_{\bar{x}_i}^2, 1 \right)_i + \left(\frac{\nu_2^{(i)}}{\Omega_i \Theta_i} y^2, 1 \right) \right], \tag{6.2}$$

where

$$\nu_2^{(i)} = \begin{cases} \frac{1}{h_i^+} \left| \kappa_i^{(1)} - \frac{\mathcal{K}_i^+}{h_i^+} + \frac{h_i^+}{4} q \right|, & x_i = 0, \\ \frac{1}{2\hbar_i} \left| \frac{\mathcal{K}_i}{h_i^-} - \frac{\mathcal{K}_i^+}{h_i^+} + \frac{\hbar_i}{2} q \right|, & x_i \neq 0, L_i, \\ \frac{1}{h_i^-} |\kappa_i^{(2)} + \frac{\mathcal{K}_i}{h_i^-} + \frac{h_i^-}{4} q|, & x_i = L_i, \ \ x_j \in \hat{\omega}_j. \end{cases}$$

Hence

$$(Dy, y) = (dy^2, 1) = \sum_{i=1}^{2} \left[\left(\Theta_i \nu_1^{(i)} y^2, 1 \right) + \left(\Omega_i \Theta_i \nu_2^{(i)} y^2, 1 \right) \right] \tag{6.3}$$

with

$$\nu_1^{(i)} = \begin{cases} \frac{\mathcal{K}_i^+}{\hbar_i h_i^+}, & x_i \neq L_i, \\ 0, & x_i = L_i, \ \ x_j \in \hat{\omega}_j. \end{cases}$$

We need the following lemma.

Lemma 6.1 *[20] Let $z(\mathbf{x})$ be the solution of the problem $\Lambda_i z = -\rho$, $x_i \in \hat{\omega}_i$ and $\Psi = 1/\max_{x \in \hat{\omega}_i(x_j)} z(\mathbf{x})$. Then*

$$\Psi(\rho y, y)_{\hat{\omega}_i(x_j)} \leq (\mathcal{K}_i y_{\bar{x}_i}^2, 1)_{\omega_i^+(x_j)} + \frac{1}{2}(qy, y)_{\hat{\omega}_i(x_j)} \kappa_i^{(1)} y^2(0, x_j) + \kappa_i^{(2)} y^2(L_i, x_j), \ \ \forall x_j \in \hat{\omega}_j.$$

Let

$$\zeta_i^{(1)} \equiv \zeta_i^{(1)}(x_j) = \max_{x_i \in \hat{\omega}_i(x_j)} y_1^{(i)}(x), \ \ \zeta_i^{(2)} \equiv \zeta_i^{2)}(x_j) = \max_{x_i \in \hat{\omega}_i(x_j)} y_2^{(i)}(x), \tag{6.4}$$

where for fixed values of $x_j \in \hat{\omega}_j$ the grid functions $y_1^{(i)}(x)$ and $y_2^{(i)}(x)$ are the solutions of three-point boundary problems

$$\Lambda_i y_1^{(i)} = -\nu_1^{(i)} \ \text{ and } \Lambda_i y_2^{(i)} = -\nu_2^{(i)}$$

respectively.

Since the grid functions Ω_i and Θ_i do not depend on x_i, we get the following inequalities

$$(\Omega_i\Theta_i\nu_2^{(i)}y^2,1) \le (\zeta_i^{(2)}\Omega_i\Theta_i\mathcal{K}_i y_{\bar{x}_i},1)_i + \frac{1}{2}(\zeta_i^{(2)}\Omega_i\Theta_i q y^2,1) + (\zeta_i^{(2)}\Omega_i\Theta_i\kappa_i^{(1)}y^2,1)_{\hat{\omega}_j(0)} + (\zeta_i^{(2)}\Omega_i\Theta_i\kappa_i^{(2)}y^2,1)_{\hat{\omega}_j(L_i)} \tag{6.5}$$

$$\left(\frac{\nu_2^{(i)}}{\Omega_i\Theta_i}y^2,1\right) \le \left(\frac{\zeta_i^{(2)}\mathcal{K}_i}{\Omega_i\Theta_i}y^2_{\bar{x}_i},1\right)_i + \frac{1}{2}\left(\frac{\zeta_i^{2)}}{\Omega_i}\frac{q}{\Theta_i}y^2,1\right) + \left(\frac{\zeta_i^{2)}\kappa_i^{(1)}}{\Omega_i\Theta_i}y^2,1\right)_{\hat{\omega}_j(0)} + \left(\frac{\zeta_i^{(2)}\kappa_i^{(2)}}{\Omega_i\Theta_i}y^2,1\right)_{\hat{\omega}_j(L_i)}, \tag{6.6}$$

$$\left(\Theta_i\nu_1^{(i)}y^2,1\right) \le \left(\zeta_i^{(1)}\Theta_i\mathcal{K}_i y^2_{\bar{x}_i}\right)_i + \frac{1}{2}\left(\zeta_i^{(1)}\Theta_i q y^2,1\right) + \left(\zeta_i^{(1)}\Theta_i\kappa_i^{(1)}y^2,1\right)_{\hat{\omega}_j(0)} + \left(\zeta_i^{(2)}\Theta_i\kappa_i^{(1)}y^2,1\right)_{\hat{\omega}_j(L_i)}. \tag{6.7}$$

If we choose Θ_i in the form

$$\Theta_i(x_j) = \left[\zeta_i^{(2)}(x_j)\Omega_i(x_j) + \zeta_i^{(1)}(x_j)\right]^{-1}, \tag{6.8}$$

and take into account (6.1), then substituting (6.5) and (6.7) into (6.3) we confirm that

$$(Dy,y) \le (Ay,y),$$

and hence in inequalities (5.6) we can set

$$\delta = 1. \tag{6.9}$$

Now we shall find the expression for Δ. Substituting (6.6) into (6.2) and taking into account (6.8) we get the following estimate

$$\left(A_1D^{-1}A_2y,y\right) \le \sum_{i=1}^{2}\left[\left((\frac{\zeta_i^{(2)}}{\Omega_i}+1)(\zeta_i^{(2)}\Omega_i+\zeta_i^{(1)})\mathcal{K}_i y^2_{\bar{x}_i},1\right)_i + \frac{1}{2}\left(\frac{\zeta_i^{(2)}}{\Omega_i}(\zeta_i^{(2)}\Omega_i+\zeta_i^{(1)})qy^2,1\right)\right.$$
$$\left. + \left(\frac{\zeta_i^{(2)}}{\Omega_i}(\zeta_i^{(2)}\Omega_i+\zeta_i^{(1)})\kappa_i^{(1)}y^2,1\right)_{\hat{\omega}_j(0)} + \left(\frac{\zeta_i^{(2)}}{\Omega_i}(\zeta_i^{(2)}\Omega_i+\zeta_i^{(1)})\kappa_i^{(2)}y^2,1\right)_{\hat{\omega}_j(L_i)}\right]. \tag{6.10}$$

Now we choose the optimal Ω_i as the solution of the following minimisation problem

$$\left(\frac{\zeta_i^{(2)}}{\Omega_i}+1\right)(\zeta_i^{(2)}\Omega_i+\zeta_i^{(1)}) \to \min,$$

i.e.

$$\Omega_i(x_j) = \sqrt{\zeta_i^{(1)}(x_j)}. \tag{6.11}$$

Hence from (6.10) we have

$$(A_1D^{-1}A_2y,y) \le \sum_{i=1}^{2}\left[\left((\zeta_i^{(2)}+\sqrt{\zeta_i^{(1)}})^2\mathcal{K}_i y^2_{\bar{x}_i},1\right)_i + \frac{1}{2}\left(\zeta_i^{(2)}(\zeta_i^{(2)}+\sqrt{\zeta_i^{(1)}})qy^2,1\right) + \left(\zeta_i^{(2)}(\zeta_i^{(2)}+\sqrt{\zeta_i^{(1)}})\kappa_i^{(1)}y^2,1\right)_{\hat{\omega}_j(0)} + \left(\zeta_i^{(2)}(\zeta_i^{(2)}+\sqrt{\zeta_i^{(1)}})\kappa_i^{(2)}y^2,1\right)_{\hat{\omega}_j(L_i)}\right].$$

This estimate together with (6.1) confirm that in inequalities (5.6) we may set

$$\Delta = 4 \max_{i=1,2} \left\{ \max_{x_j \in \hat{\omega}_j} \left[\zeta_i^{(2)}(x_j) + \sqrt{\zeta_i^{(1)}(x_j)} \right]^2 \right\}. \tag{6.12}$$

The above estimates obtained for the mixed boundary conditions of the 3rd kind. Only slight modifications are necessary in order to get analogous estimates for Dirichlet or Neumann boundary value problems.

7 Algorithmic Aspects of the Method

The algorithmic procedure for the alternating-triangular method can be derived from (5.3) with the definition of operators B and A given in Sections 5 and 6. We have

- $y_{k+1}(i_1, i_2) = y_k(i_1, i_2) - \tau_{k+1} v_k(i_1, i_2),\ i_1 = 0, ..., N_1;\ \ i_2 = 0, ..., N_2;$
- $v_k(i_1, i_2) = \beta_1(i_1, i_2) v_k(i_1 + 1, i_2) + \beta_2(i_1, i_2) v_k(i_1, i_2 + 1) + s(i_1, i_2) d(i_1, i_2) u_k(i_1, i_2),$ $i_1 = N_1 - 1, ..., 0,\ \ i_2 = N_2 - 1, ..., 0;$
- $u_k(i_1, i_2) = \alpha_1(i_1, i_2) u_k(i_1 - 1, i_2) + \alpha_2(i_1, i_2) u_k(i_1, i_2 - 1) + s(i_1, i_2) r_k(i_1, i_2),$ $i_1 = 1, ..., N_1,\ \ i_2 = 1, ..., N_2;$
- $r_k(i_1, i_2) = [r_k^{(1)}(i_1, i_2) + r_k^{(2)}(i_1, i_2)] - \varphi(i_1, i_2),\ i_1 = 0, ..., N_1,\ \ i_2 = 0, ..., N_2,$

where $\alpha_i = \omega_0 s p_2^{(i)},\ \ \beta_i = \omega_0 s \nu_1^{(i)},\ \ i = 1, 2,$

$$r_k^{(i)} = p_1^{(i)} y_k - \nu_1^{(i)} y_k^{(+1_i)} - p_2^{(i)} y_k^{(-1_i)}, s = \frac{1}{d + \omega_0 (p_1^{(1)} + p_1^{(2)})/2},$$

and

$$p_1^{(i)} = \begin{cases} \frac{2}{h_i^+} \left(\frac{\mathcal{K}_i^+}{h_i^+} + \kappa_i^{(1)} \right) + \frac{1}{2} q, & x_i = 0, \\ \frac{1}{\hbar_i} \left(\frac{\mathcal{K}_i^+}{h_i^+} + \frac{\mathcal{K}_i}{h_i^-} \right) + \frac{1}{2} q, & x_i \neq 0, L_i, \\ \frac{2}{h_i^-} \left(\frac{\mathcal{K}_i}{h_i^-} + \kappa_i^{(2)} \right) + \frac{1}{2} q, & x_i = L_i,\ x_j \in \hat{\omega}_j, \end{cases} \qquad p_2^{(i)} = \begin{cases} 0, & x_i = 0, \\ \frac{\mathcal{K}_i}{\hbar_i h_i^-} & x_i = L_i,\ x_j \in \hat{\omega}_j. \end{cases}$$

Therefore on each time layer the procedure goes as follows
Algorithm 7.1.

- compute the residual

$$r_k = A y_k - \varphi; \tag{7.1}$$

- find the auxiliary function u_k from the solution of the system of equations

$$(D + \omega_0 A_1) u_k = r_k; \tag{7.2}$$

- find the auxiliary function v_k from the system of equations

$$(D + \omega_0 A_2) v_k; \tag{7.3}$$

- compute a new approximation

$$y_{k+1} = y_k - \tau_{k+1} v_k; \tag{7.4}$$

- if $\max_{\hat{\omega}_h} |y_{k+1} - y_k| > \varepsilon$, then set $y_k = y_{k+1}$ and repeat the procedure.

We terminate the algorithm if either in all nodes of the grid $\hat{\omega}_h$ the inequality

$$|y_{k+1} - y_k| \le \epsilon$$

holds, or n_0 iterations (see Remark 5.1) have been performed. As an initial approximation we may choose any function y_0 from the space $\mathcal{H}$.

If the solution is found we may compute fluxes from (4.1) using the following difference derivatives of $\partial u/\partial x_i$

- for inner nodes:
$$\frac{\partial u}{\partial x_i} \approx \frac{h_i^+(y - y^{(-1_i)})/h_i^- + h_i^-(y^{(+1_i)} - y)/h_i^+}{2\hbar_i},$$
- for the left boundary node:
$$\frac{\partial u}{\partial x_i} \approx \frac{4u^{(+1_i)} - 3u - u^{(+2_i)}}{2h_i^+},$$
- for the right boundary node:
$$\frac{\partial u}{\partial x_i} \approx \frac{3u - 4u^{(-1_i)} + u^{(-2_i)}}{2h_i^-}.$$

Then the flux through the boundary Γ is defined as follows [10]

$$\mathcal{F}_i|_{x_i=0} = \sum_{\hat{\omega}_j} \mathcal{F}^{(i)}\hbar_j, \;\; \mathcal{F}_i|_{x_i=L_i} = -\sum_{\hat{\omega}_j} \mathcal{F}^{(i)}\hbar_j. \tag{7.5}$$

The structure of the software package is given on Figure 1. It consists of the *MAIN* program, the control program *ALTPACK* and five programs that are called from *ALTPACK* in the sequence from left to right as shown on Figure 1. Details on these programs are given in the Appendix.

8 Numerical Experiments.

The method described in the previous sections was applied to the solution of a number of problems that present interest from both theoretical and practical points of views.

• **Example 1.** We start from a linear problem in which coefficients of the equation are fast-changing functions. Such problems are typical in modelling of semiconductor devices, chemical kinetics, problems of porous media and in many other applications. Consider problem (3.1)–(3.4) in the spatial unit-square region with the Dirichlet boundary conditions ($\lambda_i^{(i)} = 0$, $\kappa_i^{(i)} = 1,\ i = 1, 2$),

$$g_1^{(1)} = \sin(4x_2),\ g_1^{(2)} = \sin(4x_2 + 4) + t^2 x_2,$$
$$g_2^{(1)} = \sin(4x_1),\ g_2^{(2)} = \sin(4x_1 + 4) + t^2 x_1.$$

and the initial condition given in the form

$$u(x_1, x_2, 0) = \sin 4(x_1 + x_2).$$

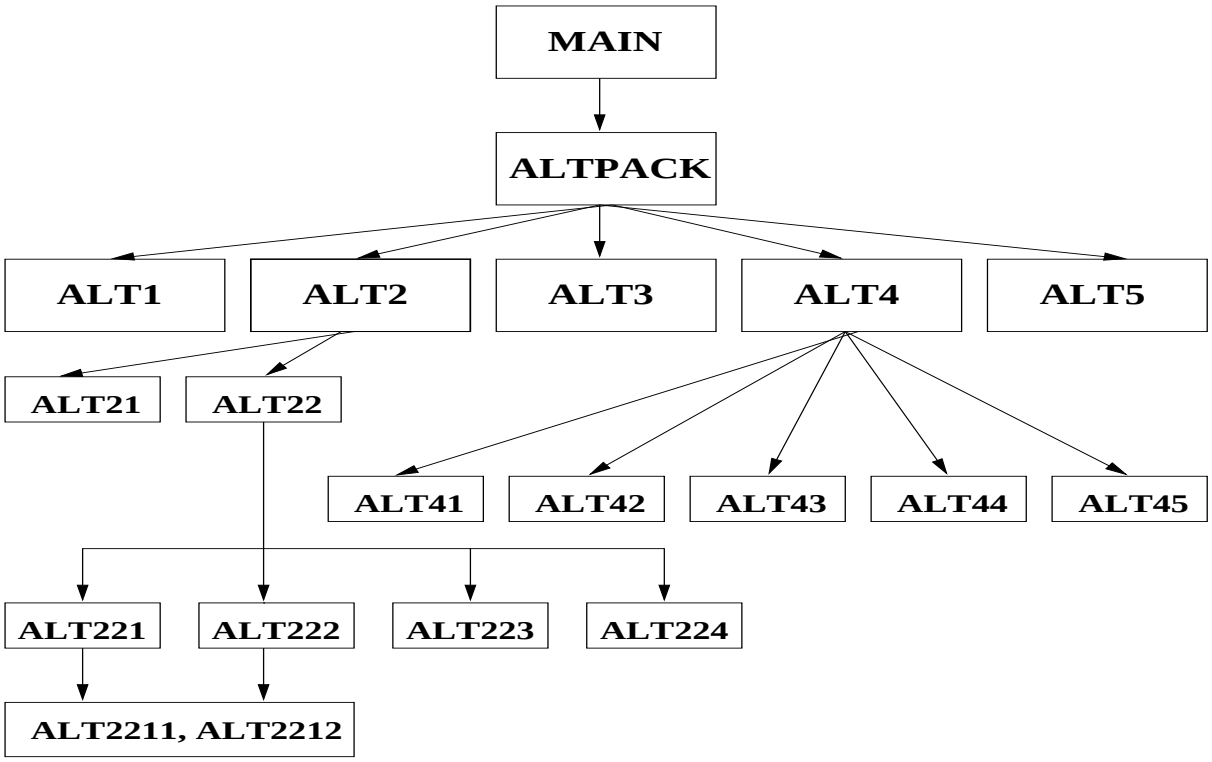

Figure 1:

Let coefficients of the equation and its right-hand side be defined as follows

$$k_1 = 1 + cx_1(1 + x_2), \quad k_2 = 1 + cx_2(1 + x_1), \quad q^0 = 0,$$

where c is a constant defined below, and

$$f^0 = 16 \sin 4(x_1 + x_2)\,[cx_1(1 + x_2) + cx_2(1 + x_1) + 2] - 4c \cos 4(x_1 + x_2)\,[x_1 + x_2 + 2] - ct^2\,[x_2(1 + x_2) + x_1(1 + x_1)] + 2tx_1x_2.$$

From the choice of the coefficients $k_i(x)$ follows that

$$c' = \min_{\mathbf{x}} k_i(\mathbf{x}) = 1 \ \text{ and } \ c'' = \max_{\mathbf{x}} k_i(\mathbf{x}) = 1 + 2c.$$

We investigated the dependency of the number of ATM iterations on the ratio $\mathcal{C} = c''/c'$. In this example we used a uniform grid with $N_1 = N_2 = 80$. The results are given in the table

below.

$\mathcal{C}$	Δ **(DB)**	$n_0(\epsilon = 1.010^{-5})$	$n_0(\epsilon = 1.010^{-7})$
2^0	138.922	15	21
2^1	197.437	17	23
2^2	309.474	19	25
2^3	557.979	21	29
2^4	1017.03	25	34
2^5	1836.22	29	39
2^6	3191.87	33	45
2^7	5131.17	37	51
2^8	7358.03	40	56

It is clear that the number of iterations for the ATM, n_0, weakly dependent on the ratio $\mathcal{C} = c''/c'$ for the values of ϵ within the range of practical applications. We computed the solution for $\mathcal{C} = 32$. It can be verified that the function

$$u(x_1, x_2, t) = \sin 4(x_1 + x_2) + t^2 x_1 x_2 \tag{8.1}$$

provides the analytical solution to the above problem. Our results do not deviate from the exact solution (8.1) for more than $\sim 10^{-4}$. On Figure 2 we present the solution for $t = 0.01$, $t = 1.2$ and $t = 5$. We see that the "upper tongue" of the solution grows steadily that indicates an increasing contribution of the second term from (8.1). Finally this term becomes dominant that is confirmed by the lower left plot. The typical structure of the solution error is shown on the lower right plot of Figure 2.

The situation when coefficients of the differential equation change locally very rapidly is typical in many applications such as semiconductor device modelling and chemical kinetics [15]. Although spectra boundaries may not change drastically, large values of the ratio $\mathcal{C} = c''/c'$ cause serious mathematical difficulties for the solution of such problems. The proposed method allows us to overcome some such difficulties due to a weak dependency of its quality on the increase of such a ratio.

• **Example 2.** In this example we consider a power-type of coefficient nonlinearities in (3.1)

$$\frac{\partial u}{\partial t} = \sum_{i=1}^{2} \frac{\partial}{\partial x_i} \left(k_i(u) \frac{\partial u}{\partial x_i} \right), \tag{8.2}$$

with $k_1(u) = k_2(u) = u^\sigma$. Equation (8.2) is a two-dimensional analogue of self-similar $S-$regime considered in [21]. We choose the initial condition in the "peaking" form

$$u(x_1, x_2, 0) = 0.5 T_f^{-1/\sigma} \left(1 - \sum_{i=1}^{2} \frac{\xi_i x_i}{\Xi} \right)_+^{2/\sigma}, \tag{8.3}$$

where

$$(z)_+ = \max(z, 0), \quad \Xi = \sqrt{2(0.5)^\sigma \frac{\sigma + 2}{\sigma}}.$$

For $x_1 = 0$ and $x_2 = 0$ the boundary conditions were defined from the following majorant

$$u(x_1, x_2, t) = 0.5 (T_f - t)^{-1/\sigma} \left(1 - \sum_{i=1}^{2} \frac{\xi_i x_i}{\Xi} \right)_+^{2/\sigma}. \tag{8.4}$$

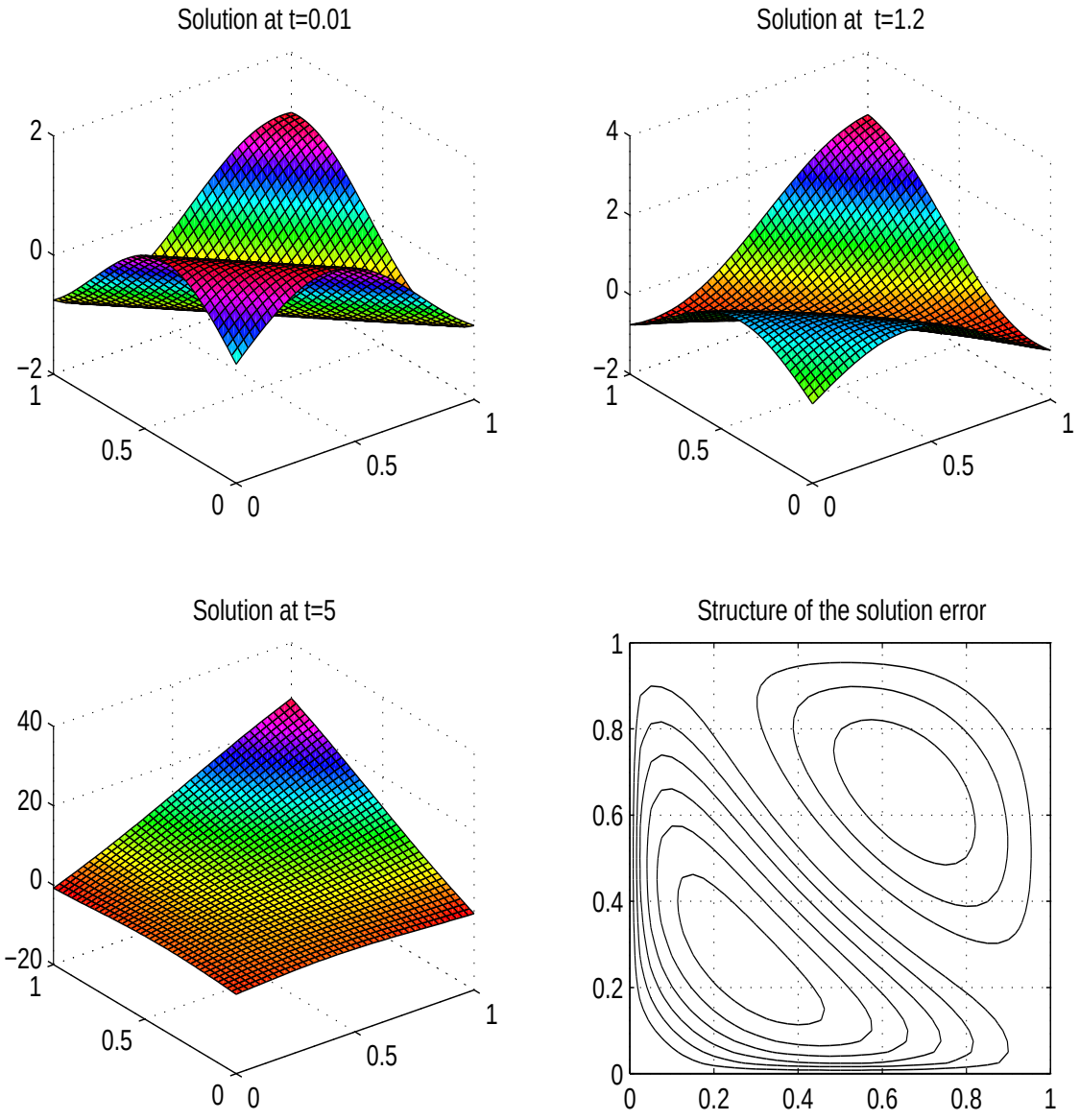
Solution at t=0.01
Solution at t=1.2
Solution at t=5
Structure of the solution error

Figure 2:

Namely, the computation was conducted for

$$u(x_1, 0, t) = 0.5(T_f - t)^n \left(1 - \frac{\xi_1 x_1}{\Xi}\right)_+^{2/\sigma}, \tag{8.5}$$

$$u(0, x_2, t) = \frac{1}{2}(T_f - t)^n \left(1 - \frac{\xi_2 x_2}{\Xi}\right)_+^{2/\sigma} \tag{8.6}$$

with the constants $T_f = 1,\ \Xi = 1, \xi_1 = \xi_2 = 1/\sqrt{2}$. On other two sides of the region boundary zero-flux conditions were assumed.

We note (see details in [21]) that the majorant function (8.4) for boundary conditions (8.5) and (8.6) defines the boundary temperature on the axes x_1 and x_2 as zero whenever $x_1 \geq \Xi/\xi_1, x_2 \geq \Xi/\xi_2$. The temperature increases with peaking when $0 \leq x_1 \leq \Xi/\xi_1$, $0 \leq x_2 \leq \Xi/\xi_2$.

First we consider the case when $n < -1/\sigma$ (HS-regime according to the classification given in [21]). In our experiment we have chosen $n = -1$ and $\sigma = 2$. From the initial moment of time to a certain finite time qualitative picture of the process remains the same. We observe a two-dimensional standing thermal wave shown on the left upper plot of Figure 3. The thermal energy of such a wave is in a finite region of heat localisation defined by a triangle with vertices $(0, 0)$, $(\sqrt{2}, 0)$, and $(0, \sqrt{2})$. In other parts of the region temperature remains zero during a finite period of time. When such time elapses, the profile of the standing wave starts to change gradually, indicating the movement of the thermal wave. The interface between the region of heat "localisation" and the region with zero-temperature distorts (see upper right plot), and we finally observe the solution blow-up in finite time when $t \to T_f^-$. On lower plots of Figure 3 the solution and its contour lines in $(x_1 x_2)$ plane are presented for the moment $t = 0.99$.

In order to obtain this solution on the mesh 41×41 it was necessary to conduct 62 ATM iteration. The computation required 10 non-linear iterations and Δ was equal 11497.5.

For the case $n > -1/\sigma$ (LS-regime according to the classification given in [21]) the qualitative behaviour of the solution remains similar to the situation described above. However, the change of the temperature profile and deterioration of the "localisation" region begins essentially later compared to the case $n < -1/\sigma$. The results are presented on Figure 4. For $n = -0.25$ and $\sigma = 2$ it was necessary to perform 36 ATM iterations and the same number of nonlinear iterations in order to obtain the solution on the mesh 41×41. In this case Δ was equal 1280.65.

• **Example 3.** In this example we investigate the behavior of "thermal crystals" produced by thermal energy localised in certain space regions [21]. In the region Q_T we consider equation (8.2) with the initial condition (8.3). As above, the initial temperature distribution is localised in a region

$$\alpha_1|x_1| + \alpha_2|x_2| \leq \Xi, \quad \text{where } \alpha_1^2 + \alpha_2^2 = 1. \tag{8.7}$$

However now we assume zero-flux conditions on the boundary of the region G, i.e. in (3.3), (3.4) we set

$$\lambda_i^{(i)} = 1, \quad \kappa_i^{(i)} = 0, \quad g_i^{(i)} = 0, \ i = 1, 2. \tag{8.8}$$

Figure 5 demonstrates some results of our investigations. Initially thermal energy is localised in the square region $[-\sqrt{2}, \sqrt{2}] \times [-\sqrt{2}, \sqrt{2}]$ (upper left plot). When time progresses the temperature profile becomes more and more convex (upper right plot). When the thermal wave starts moving, the region of heat localisation is also transformed acquiring oval outlines

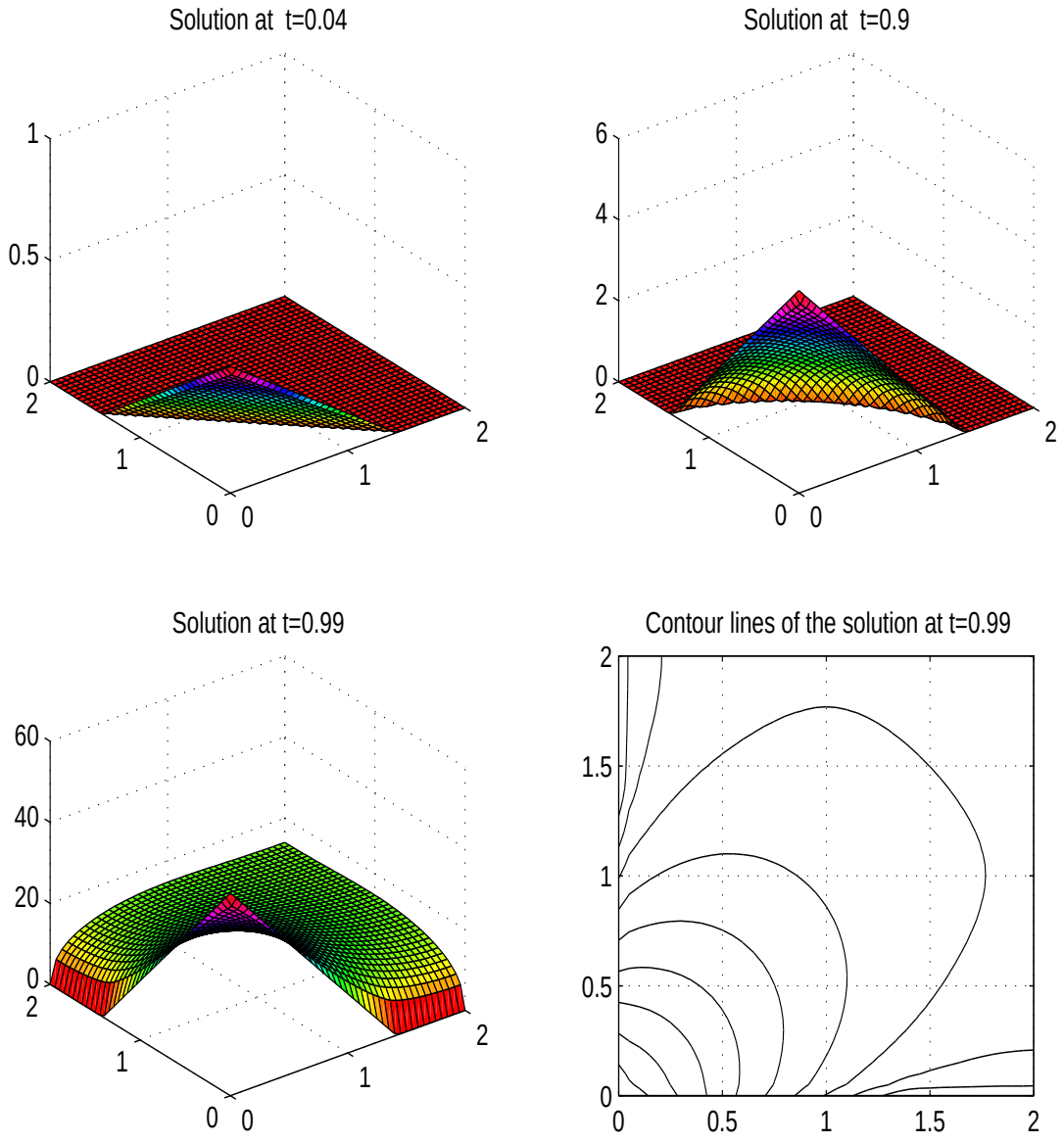
Solution at t=0.04
Solution at t=0.9
Solution at t=0.99
Contour lines of the solution at t=0.99

Figure 3:

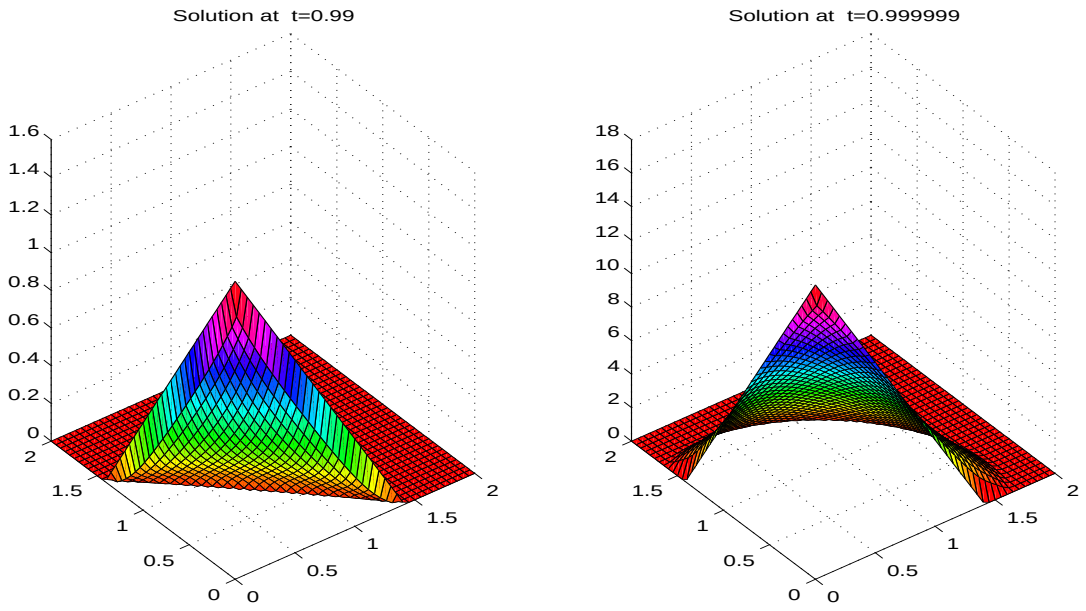

Figure 4:

(see lower right plot). The time of existence of such thermal crystals may be estimated from below [21]

$$t_{loc} \geq \frac{\sigma \Xi^2}{2(\sigma+2)(0.5)^\sigma}. \tag{8.9}$$

For $\sigma = 2$ and $\Xi = 1$ the estimate (8.9) gives $t_{loc} \geq 1$. When $t = 1$ we needed 9 ATM iterations. In this case Δ equal 3.39866.

• **Example 4.** In the concluding example we consider the equation

$$\frac{\partial u}{\partial t} = \Delta u^m \pm u^p. \tag{8.10}$$

First we consider problem (8.10) with a positive source where $m = 2,\ p = 2$. The problem is supplemented by the initial condition

$$u(x_1, x_2, 0) = (x_1 - 1)^2 + (x_2 - 1)^2. \tag{8.11}$$

Boundary conditions for (8.10) coincide with the boundary conditions of Example 2.

Figure 6 presents the results on the evolution of the thermal-wave solution which exhibits the blow-up behaviour when $t \to T_f^-$. We note that the computational complexity is essentially increases when $t \to T_f^-$. For example, to compute the solution on the mesh 41×41 for $t = 0.01$ we needed only 14 ATM iterations ($\Delta = 27.9721$). When $t = 0.97$ the number of ATM iterations increases to 70 ($\Delta = 18856.5$) and the process requires 25 nonlinear iterations.

We also considered the problem (8.10) with absorption where $m = 2,\ p = 0.5$.The initial condition was defined by (8.11) and no-flux boundary conditions were assumed.

Figure 7 demonstrates the solution quenching in finite time. The theoretical investigation of such a solution and the conditions on the existence of its non-trivial continuation after the onset of extinction are given in [5].

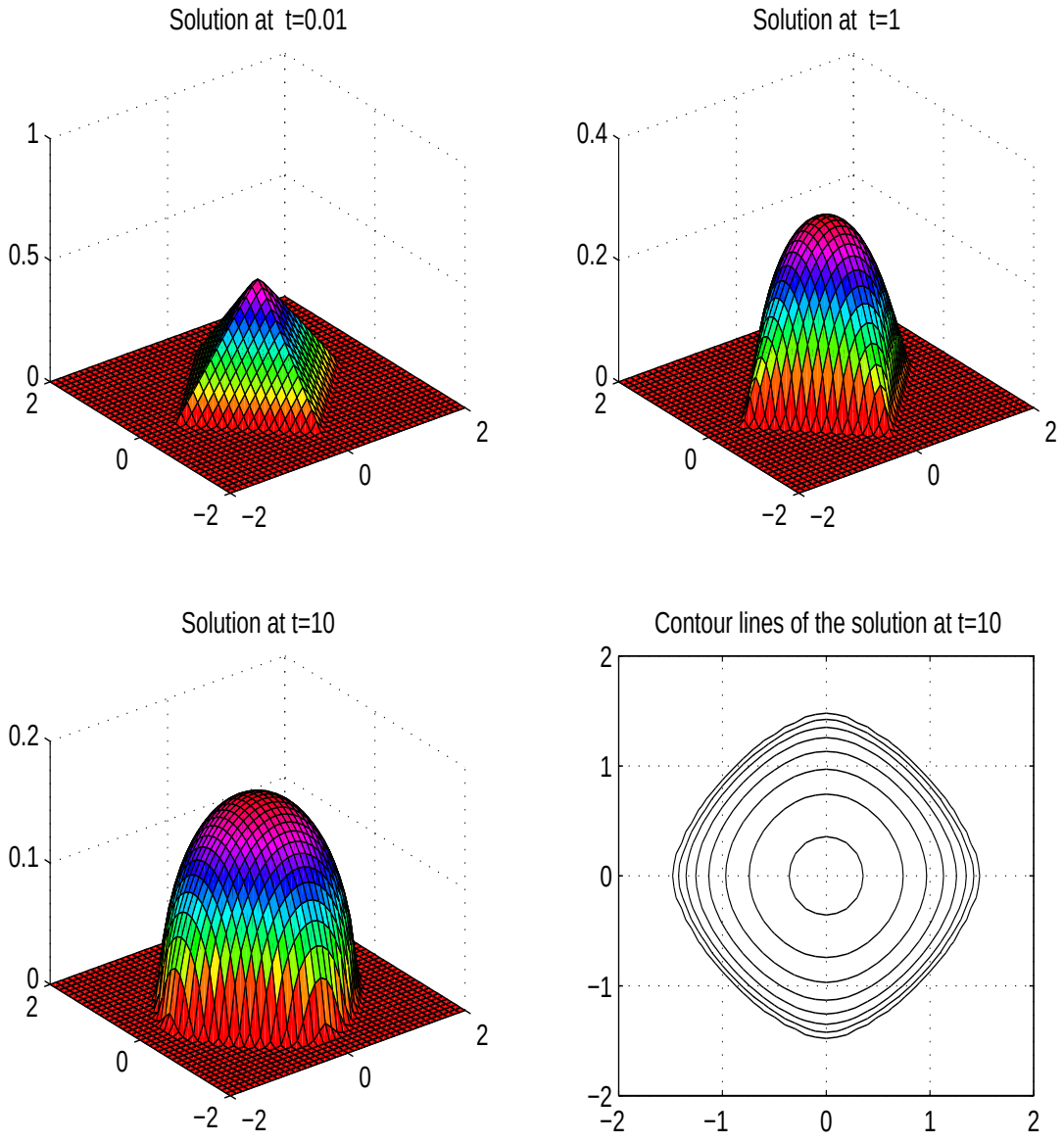
Solution at t=0.01
Solution at t=1
Solution at t=10
Contour lines of the solution at t=10

Figure 5:

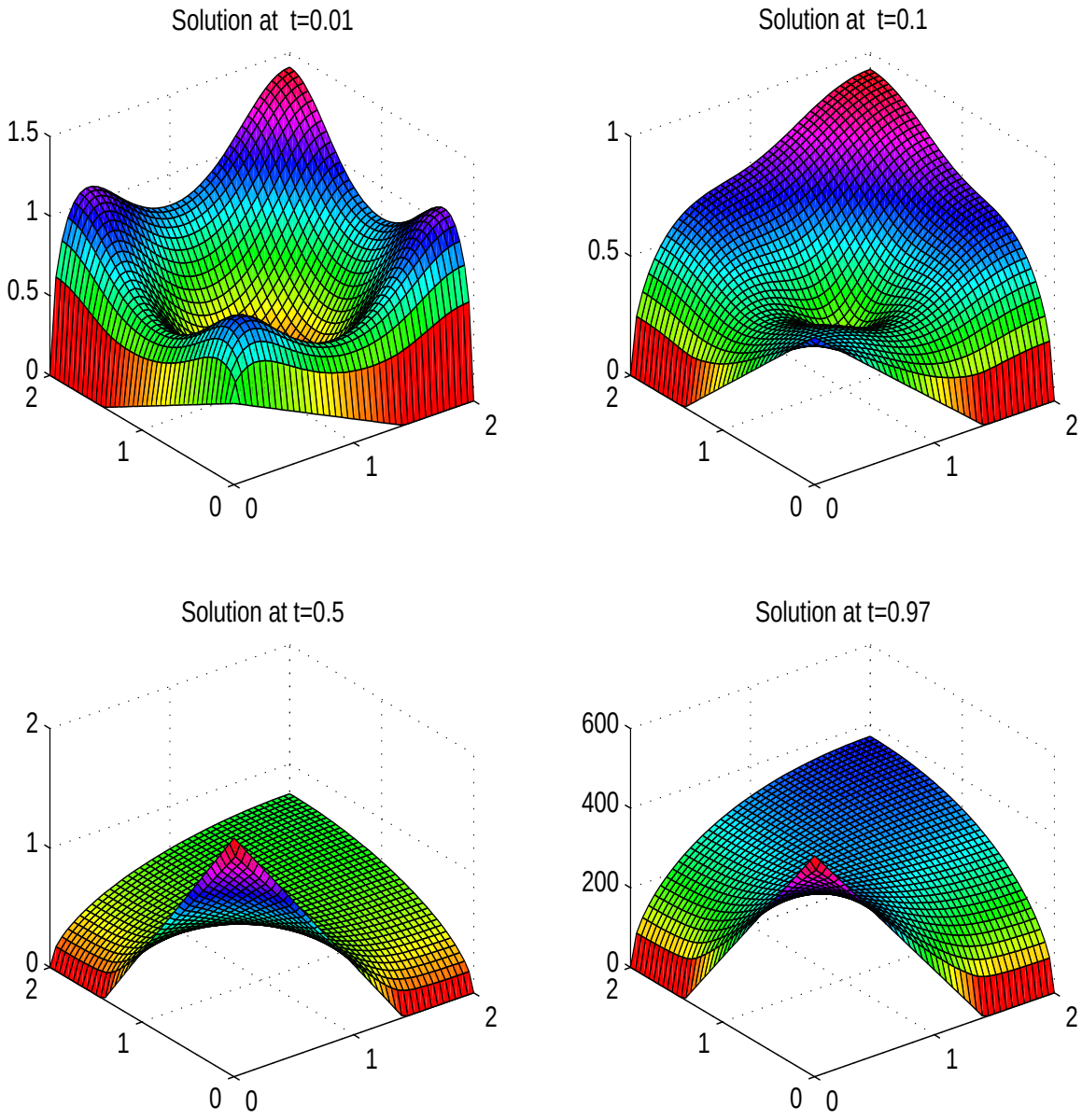
Solution at t=0.01
Solution at t=0.1
Solution at t=0.5
Solution at t=0.97

Figure 6:

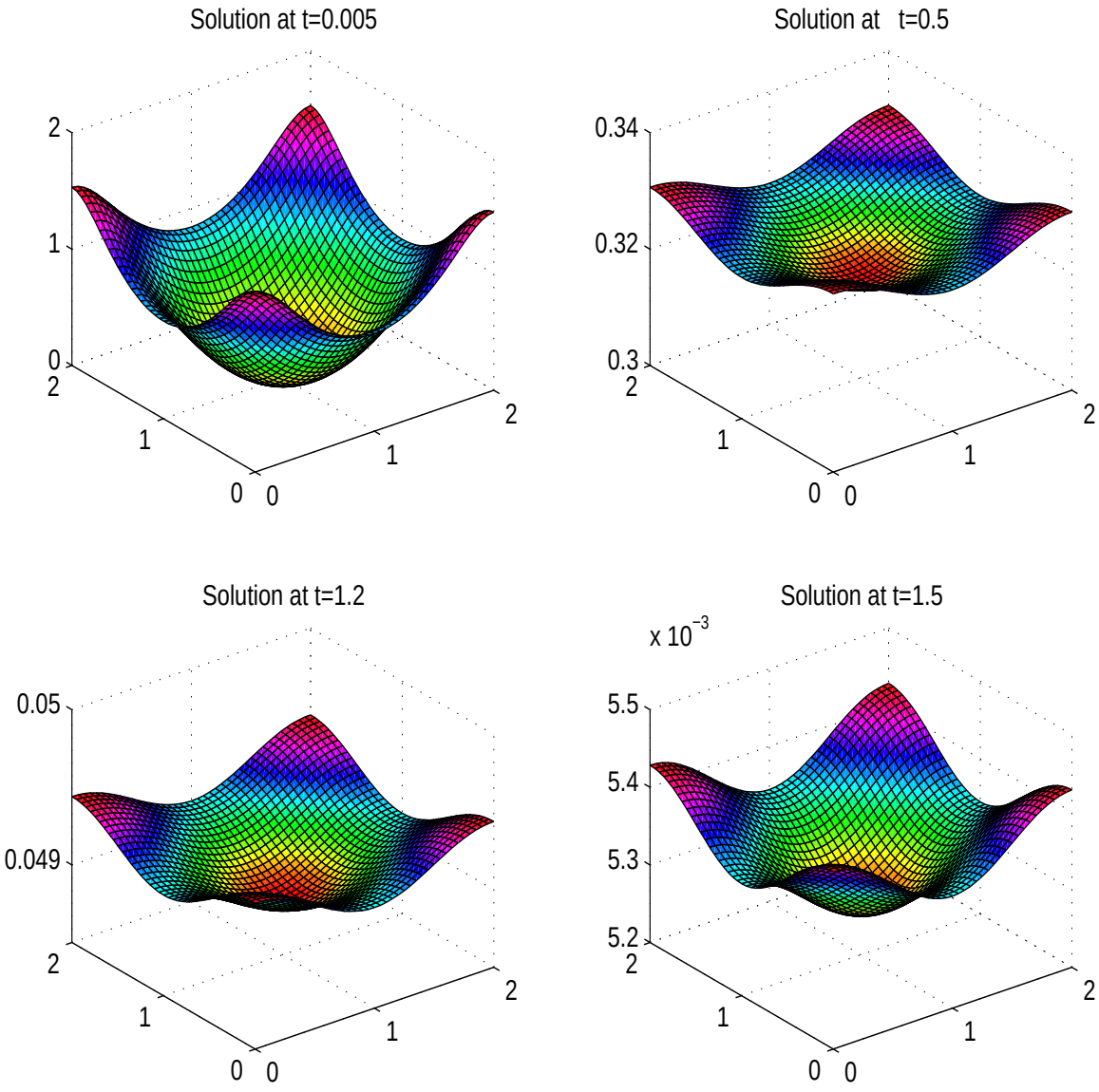
Solution at t=0.005
Solution at t=0.5
Solution at t=1.2
Solution at t=1.5
x 10^-3

Figure 7:

9 Conclusion

In this paper we described an effective procedure for the solution of nonlinear (and linear) parabolic and elliptic equations in the two-dimensional case. We showed the effectiveness of the method for the problems with fast-changing coefficients as well as for the problems with different types of nonlinearities. Blow-up and quenching phenomena were investigated using the software package ALTPACK that implements the alternating-triangular method.

In the program ALTPACK we applied the procedure of ordering for Chebyshev iterative parameters. This allowed us to minimise the influence of round-off errors and to eliminate large intermediate values (that are dependent on the number of iterations $n(\epsilon)$) in the computational procedure. For a number of non-linear problems ALTPACK shows better results than the classical implicit methods of alternating directions [12, 18]. It is also known that for model problems [19, 20] both methods, ATM and ADI, require the same number of iterations but on average the ATM requires less arithmetic operations. Finally the ATM is easily implemented for parallel and vector computation.

Acknowledgements

The work was supported by grant USQ-PTRP 179389. The author is grateful to Ross Darnell and Harry Butler for their helpful assistance at the final stage of preparation of this paper.

References

[1] Bai, C., Lavin, A.S., On hyperbolic heat conduction and the second law of thermodynamics, *ASME J. of Heat Transfer,* **117**, 1995, 256–263.

[2] Bebernes, J., Eberly, D., Mathematical Problems from Combustion Theory, Springer-Verlag, 1989.

[3] Fleming, W. and Soner, H., *Controlled Markov Processes and Viscosity Solutions,* Springer-Verlag, 1993.

[4] Fujita, H., and Suzuki, T. Evolution problems, *in "Handbook of Numerical Analysis", Ed. P.G. Ciarlet & J.L Lions,* North-Holland, Amsterdam, New York, Oxford, Tokyo, 1991, Vol. II, 789-923.

[5] Galaktionov, V.A., Vazquez, J.L., Continuation of Blowup Solutions of Nonlinear Heat Equations in Several Space Dimensions, *Comm. on Pure and Appl. Math.,* Vol. L, 1997, 1-67.

[6] Goncharenko, V.M., Lychman, V.V., Numerical Solution of a Boundary-Value Problem of Elasticity Theory for a Body with an Inclusion, *J. Math. Sci.,* **72**, No.3, 1994, 3116–3119.

[7] Hageman, L.A., Young, D.M., *Applied Iterative Methods,* Academic Press, 1981.

[8] Levine, H., The role of critical exponents in blowup theorems, *SIAM Review,* Vol. 32, No. 2, 1990, 262–288.

[9] Logan, J.D., *An Introduction to Nonlinear Partial Differential Equations,* Wiley & Sons, 1994.

[10] Lychman, V.V., Mistetskij, G.E., Numerical Solution of Subsurface Moisture Transport Problems, *Journal of S. Math.,* **54**, No. 2, 1991, 824–831.

[11] Makarenko, A.S., Mathematical Modeling of Heat-Distribution Processes using Generalized Equations for Thermal Conductivity, *J. of Math. Sciences,* Vol. 70, No. 1, 1994, 1529–1533.

[12] Melnik, R.V.N., Correction for Nonstationarity and Internal Nonlinearity in the Analysis of Integrated-Circuit Thermal Parameters, *Radioelectronics & Communications Systems (Alerton Press)*, Vol. 34, No. 6, 1991, 84–86.

[13] Melnik, R.V.N., Discrete Models of Coupled Dynamic Thermoelasticity for Stress-Temperature Formulations, submitted to *Mathematical Problems in Engineering: TMA* (Preprint SC-MC-9703, Dept. of Math. & Comp., University of Southern Queensland).

[14] Melnik, R.V.N., The Stability Condition and Energy Estimate for Nonstationary Problems of Coupled Electroelasticity, *Mathematics and Mechanics of Solids,* 2, 1997, 153–180.

[15] Melnik, R.V.N., Melnik, K.N., Modelling of Nonlocal Physical Effects in Semiconductor Plasma Using Quasi-Hydrodynamic Models, *Computational Techniques and Applications: CTAC97,* World Scientific, 1998.
[16] Morton, K.W., *Numerical Solution of Convection-Diffusion Problems,* Chapman & Hall, 1996.
[17] Muller, I., Ruggeri, T., *Extended Thermodynamics,* Springer-Verlag, 1993.
[18] Ortega, J.M., *Introduction to Parallel and Vector Solution of Linear Systems,* Plenum Press, New York, 1988.
[19] Samarskii, A.A., *Theorie der Differenzenverfahren,* (Series: Mathematik und ihre Anwendungen in Physik und Technik), Aufl. Leipzig: Academische Verlagsgesellschaft Geest & Portig, 1984.
[20] Samarskii, A.A., Nikolaev, E.S., *Numerical Methods for Grid Equations,* Basel, Boston: Birkhauser Verlag, 1989.
[21] Samarskii, A.A. et al, *Blow-up in Quasilinear Parabolic Equations,* Vol. 19, de Gruyter Expositions in Mathematics, de Gruyter, Berlin and Hawthorne, NY, 1995.
[22] Shashkov, M., Steinberg, S., Conservative Finite-Difference Methods on General Grids, *Boca Raton: CRC Press,* 1995.
[23] Vladimirov, V.S., *Equations of Mathematical Physics,* Moscow, Mir, 1984.

Appendix

Subroutines	Calling Source	Functions/Description
ALTPACK	MAIN	Solution of time-dependent (or stationary) problems for nonlinear (or linear) PDEs
ALT1	ALTPACK	Preparation of initial information for the region discretisation
ALT2	ALTPACK	Preparation of initial information for the ATM; call ALT21, ALT22
ALT3	ALTPACK	Construction of the optimal ordered set of Chebyshev iterative parameters
ALT4	ALTPACK	Solution of the discrete problem by the ATM; call ALT41, ALT42, ALT43, ALT44, ALT45
ALT5	ALTPACK	Print the results for graphics post-processing
ALT21	ALT2	Computation of grid functions for the discrete problem
ALT22	ALT2	Computation of *a priori* information for the ATM (call ALT221, ALT222, ALT223, ALT224
ALT41	ALT4	Formation of the discrete problem (construction of the grid functions in the left hand side of the system)
ALT42	ALT4	Construction of the right hand side of the system of grid equations
ALT43	ALT4	Solution of the linear system of discretised equations
ALT44	ALT4	Verification of the convergence of nonlinear iterations
ALT45	ALT4	Verification of stopping criteria
ALT221	ALT22	Preparation of the information for the sweeping algorithm in the x_1-direction
ALT222	ALT22	Preparation of the information for the sweeping algorithm in the x_2-direction
ALT223	ALT22	Computation of operator bounds required as *a priori* information for the problem
ALT224	ALT22	Computation of grid functions required for the definition of the system of discretised equations (such functions are used in ALT41)
ALT2211	ALT221, ALT222	Solution of discretised equations by the left sweeping algorithm
ALT2212	ALT221, ALT222	Solution of the discretised equations by the right sweeping algorithm