

NUMERICAL SOLUTION OF REACTION-DIFFUSION EQUATIONS

Jan Lamac̃

Technical University of Liberec
Faculty of Science, Humanities and Education
Department of Mathematics and Didactics of Mathematics
Studentská 2, 461 17, Liberec, Czech Republic

*Charles University in Prague
Faculty of Mathematics and Physics
Department of Numerical Mathematics
Sokolovská 83, Praha 8, 186 75, Czech Republic

**Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering
Břehová 7, 115 19 Praha, Czech Republic
jan.lamac@centrum.cz

Abstract

The subject of the presented paper is a mathematical analysis and numerical solution of the system of nonlinear nonstationary reaction-diffusion equations. Firstly, using the invariant region technique, the proof of both the existence and uniqueness of the solution and problem data continuous dependence is carried out. After time discretization of the problem the Galerkin finite elements method is applied and a priori error estimates of the method are derived. A suitable mesh adaptivity is discussed as well. The method is finally implemented and tested on several examples.

Keywords: Invariant region; reaction; diffusion; finite elements method; adaptivity.

Introduction

Reaction-diffusion equations provide an efficient mathematical model for description of changes in concentration of one or more substances under an influence of two basic physical (and chemical) processes - diffusion and reaction. Using these equations one can also describe several mechanisms that occur in nature (see [5]). One of them is the evolution of bacteria populations.

Let us denote $u_i = u_i(x, t)$, $i = 1, 2, \dots, N$, concentrations of N types of bacteria at time t and place x , then the mathematical model of the evolution of bacteria populations is described by the system of nonlinear nonstationary reaction-diffusion equations (see [6],[7],[8])

$$\frac{\partial u_i}{\partial t} = D_i \Delta u_i + \left(r_i - \sum_{j=1}^N a_{ij} u_j \right) u_i, \quad \text{in } Q_T, \quad i = 1, 2, \dots, N, \quad (1)$$

where $Q_T = \Omega \times (0, T)$ and $D_i, r_i > 0, a_{ij} \geq 0$ are given constants. For each function u_i , $i = 1, 2, \dots, N$, we also prescribe initial and boundary conditions

$$u_i(x, 0) = u_{0i}(x) \quad \text{in } \Omega, \quad (2)$$

$$\frac{\partial u_i}{\partial \mathbf{n}} = g_i \quad \text{on } \Gamma_N \times (0, T), \quad (3)$$

$$u_i = u_{Di} \quad \text{on } \Gamma_D \times (0, T), \quad (4)$$

where $\mathbf{u}_0 : \Omega \rightarrow \mathbb{R}^N$, $\mathbf{g} : \Gamma_N \times (0, T) \rightarrow \mathbb{R}^N$ and $\mathbf{u}_D : \Gamma_D \times (0, T) \rightarrow \mathbb{R}^N$ are given functions and Γ_N, Γ_D are parts of the boundary $\partial\Omega$ such that $\overline{\Gamma_N \cup \Gamma_D} = \partial\Omega$ and $\Gamma_N \cap \Gamma_D = \emptyset$.

1 Weak Formulation

Let us denote $I = (0, T)$ and suppose that for each $i = 1, 2, \dots, N$, there exist functions $\tilde{u}_{Di} \in L^2(I, H^1(\Omega)) \cap L^\infty(I, L^2(\Omega))$ with $\tilde{u}'_{Di} \in L^2(I, H^{-1}(\Omega))$ such that for almost all $t \in I$ holds $\tilde{u}_{Di}(t)|_{\Gamma_D} = u_{Di}(t)$ in the sense of traces. Further, let $g_i \in L^2(I, L^2(\Gamma_N))$ and $u_{0i} \in L^2(\Omega)$ for each $i = 1, 2, \dots, N$ and in order to exclude trivial solutions let us also suppose that for each $i = 1, 2, \dots, N$, one has $\|u_{0i}\|_2 \geq m_i > 0$.

If we then define $V = \{v \in H^1(\Omega) \mid v = 0 \text{ on } \Gamma_D \text{ in the sense of traces}\}$, we call $\mathbf{u} \in L^\infty(I, L^2(\Omega))^N \cap L^2(I, H^1(\Omega))^N$ the weak solution of the problem (1) provided that for each $i = 1, 2, \dots, N$, holds

- $\frac{du_i}{dt} \in L^2(I, V^*)$,
- $u_i(0) = u_{0i}$,
- $u_i(t) - \tilde{u}_{Di}(t) \in V$ for almost all $t \in I$
- and for each $v \in V$ and almost all $t \in I$ holds

$$\left(\frac{du_i}{dt}(t), v\right) + D_i(\nabla u_i(t), \nabla v) = \left(\left(r_i - \sum_{j=1}^N a_{ij}u_j(t)\right)u_i(t), v\right) + D_i(g_i, v)_{\Gamma_N}.$$

This formulation can be easily derived using integration and Green's theorem.

2 Existence and Uniqueness

The existence and uniqueness of the solution of the problem (1) follow from the boundedness of this solution. The boundedness of the solution of the problem (1) can be proved by construction of the *invariant region* (see [4] or [10]).

Definition 1. *The invariant region of the problem (1) is every closed set $\Sigma \subset \mathbb{R}^N$ with the property*

$$\mathbf{u}_0, \mathbf{u}_D \in \Sigma \text{ for all } t \in [0, T], x \in \Omega \Rightarrow \mathbf{u}(x, t) \in \Sigma \text{ for all } t \in [0, T], x \in \Omega. \quad (5)$$

Let us denote $f_i(\mathbf{z}) = \left(r_i - \sum_{j=1}^N a_{ij}z_j\right)z_i$. If one wants to certify that Σ is the invariant region of the problem (1), it is sufficient (see [10]) to prove that for each $\mathbf{z} \in \partial\Sigma$ the vector $\mathbf{f}(\mathbf{z})$ points inside the set Σ . Considering $a_{ii} > 0$ for each $i = 1, 2, \dots, N$, we can define $\Sigma = \times_{i=1}^N [0, M_i]$, where $M_i > \max\{\|u_{0i}\|_\infty, \|u_{Di}\|_\infty, r_i/a_{ii}\}$. Consequently, for every $\mathbf{z} \in \partial\Sigma$ there exists $i \in \{1, 2, \dots, N\}$ such that $z_i = 0$ or $z_i = M_i$ and thus we can denote $\mathbf{z}^{iL}, \mathbf{z}^{iR} \in \partial\Sigma$ such that $z_i^{iL} = 0$ and $z_i^{iR} = M_i$. Finally, it is obvious, that vectors $\mathbf{f}(\mathbf{z}^{iL}), \mathbf{f}(\mathbf{z}^{iR})$ points inside the set Σ if and only if $f_i(\mathbf{z}^{iL}) > 0$ and $f_i(\mathbf{z}^{iR}) < 0$. In the second case one has

$$f_i(\mathbf{z}^{iR}) = \left(r_i - \sum_{\substack{j=1 \\ j \neq i}}^N a_{ij}z_j^{iR} - a_{ii}M_i\right)M_i < -M_i \sum_{\substack{j=1 \\ j \neq i}}^N a_{ij}z_j^{iR} \leq 0, \quad (6)$$

while in the first case holds

$$f_i(\mathbf{z}^{iL}) = \left(r_i - \sum_{\substack{j=1 \\ j \neq i}}^N a_{ij}z_j^{iL} - a_{ii} \cdot 0\right) \cdot 0 = 0. \quad (7)$$

Thus the vector $\mathbf{f}(\mathbf{z}^{iL})$ is tangent to $\partial\Sigma$ and does not points inside the set Σ . Nevertheless, this drawback can be removed by showing that the problem (1) is f -stable.

Definition 2. We call the problem (1) f -stable, if there exists a sequence of functions $\{\mathbf{f}_m\}_{k=1}^\infty$ such that $\|\mathbf{f} - \mathbf{f}_m\|_{\mathcal{C}^1(\Sigma)^N} \xrightarrow{m \rightarrow \infty} 0$ implies $\|\mathbf{u} - \mathbf{u}_m\|_{\mathcal{C}^1(I, L^2(\Omega))^N} \xrightarrow{m \rightarrow \infty} 0$, where \mathbf{u} is the solution of the problem (1) with the function \mathbf{f} on the right-hand side and \mathbf{u}_m is the solution of the problem (1) with the function \mathbf{f}_m on the right-hand side.

Remark 1. The f -stability of the problem (1) can be shown using the sequence \mathbf{f}_m satisfying $f_{m,i}(\mathbf{z}) = f_i(\mathbf{z}) + \frac{\|u_{0,i}\|_2 - z_i}{m}$.

Theorem 1. (Existence, uniqueness and data continuous dependence) Let the functions $\mathbf{u}_0, \tilde{\mathbf{u}}_D$ and \mathbf{g} satisfy assumptions from the previous section. If the problem (1) is f -stable, then there exists a unique solution \mathbf{u} of the problem (1) and positive constants $B_i = B_i(T)$, $i = 1, 2, 3$, independent from \mathbf{u} , such that :

$$\sup_{t \in [0, T]} \|\mathbf{u}(t)\|_2^2 \leq B_1 \mathcal{K}(\mathbf{u}_0, \tilde{\mathbf{u}}_D, \mathbf{g}), \quad (8)$$

$$\int_0^T \|\nabla \mathbf{u}(t)\|_2^2 dt \leq B_2 \mathcal{K}(\mathbf{u}_0, \tilde{\mathbf{u}}_D, \mathbf{g}), \quad (9)$$

$$\int_0^T \|(\mathbf{u})'(t)\|_{-1,2}^2 dt \leq B_3 \mathcal{K}(\mathbf{u}_0, \tilde{\mathbf{u}}_D, \mathbf{g}), \quad (10)$$

where

$$\mathcal{K}(\mathbf{u}_0, \tilde{\mathbf{u}}_D, \mathbf{g}) = \|\mathbf{u}_0\|_2^2 + \sup_{t \in [0, T]} \|\tilde{\mathbf{u}}_D(t)\|_2^2 + \int_0^T \|\tilde{\mathbf{u}}_D'(t)\|_{-1,2}^2 + \|\tilde{\mathbf{u}}_D(t)\|_{1,2}^2 + \|\mathbf{g}(t)\|_{2, \Gamma_N}^2 dt. \quad (11)$$

Proof. Sketch of the proof: Since \mathbf{u} is bounded, $\mathbf{f}(\mathbf{u})$ is Lipschitz-continuous and the existence and uniqueness come from the Banach fix-point theorem and Gronwall's lemma respectively. Estimates (8)-(10) can be derived from the weak formulation using Young's inequality. \square

Previous theorem also implies that for sufficiently smooth data ($\mathcal{K}(\mathbf{u}_0, \tilde{\mathbf{u}}_D, \mathbf{g}) < \infty$), the solution of the problem (1) belongs to $\mathcal{C}((0, T), L^2(\Omega))$.

3 Numerical Solution

Let us choose $p \in \mathbb{N}$, denote $\tau = T/p$ and define a partition of the interval $[0, T]$: $t_k = k\tau$, for $k = 0, 1, \dots, p$. Further, let us denote $u_i^k(x) = u_i(x, t_k)$, $g_i^k(x) = g_i(x, t_k)$ and $u_{Di}^k(x) = u_{Di}(x, t_k)$, for $i = 1, 2, \dots, N$ and $k = 1, 2, \dots, p$. We also suppose $u_i^0(x) = u_{0,i}(x)$ for $i = 1, 2, \dots, N$ and approximate the time derivative using the backward difference, i.e. $u_i'(x, t_{k+1}) \approx \frac{u_i^{k+1}(x) - u_i^k(x)}{\tau}$ for $k = 0, 1, \dots, p-1$.

Then the time-discretization (see [9]) of the problem (1) reads: For each $k = 0, 1, \dots, p-1$ find a function $\mathbf{u}^{k+1} : \Omega \rightarrow \mathbb{R}^N$ such that for each $i = 1, 2, \dots, N$, holds

$$\frac{u_i^{k+1} - u_i^k}{\tau} = D_i \Delta u_i^{k+1} + \left(r_i - \sum_{j=1}^N a_{ij} u_j^k \right) u_i^{k+1} \quad \text{in } \Omega, \quad (12)$$

$$\frac{\partial u_i^{k+1}}{\partial \mathbf{n}}(x) = g_i^{k+1}(x) = g_i(x, t_{k+1}) \quad \text{on } \Gamma_N, \quad (13)$$

$$u_i^{k+1}(x) = u_{Di}^{k+1}(x) = u_{Di}(x, t_{k+1}) \quad \text{on } \Gamma_D, \quad (14)$$

where we used linearization $u_j^k u_i^{k+1} \approx u_j^{k+1} u_i^{k+1}$. Consequently, the corresponding weak formulation of the problem (12)-(14) reads: For each $k = 0, 1, \dots, p-1$ and $i = 1, 2, \dots, N$, find $u_i^{k+1} \in H^1(\Omega)$ such that

- $u_i^{k+1} - \tilde{u}_{Di}^{k+1} \in V$
- and for all $v \in V$ holds

$$\left(\frac{1}{\tau} - r_i\right)(u_i^{k+1}, v) + D_i(\nabla u_i^{k+1}, \nabla v) + \sum_{j=1}^N a_{ij}(u_j^k u_i^{k+1}, v) = \frac{1}{\tau}(u_i^k, v) + D_i(g_i^{k+1}, v)_{\Gamma_N}.$$

3.1 Finite Elements Method

Let us define the triangulation \mathcal{T}_h of the domain Ω consisting of a finite number of triangular elements K_i and satisfying $\overline{K_i} \cap \overline{K_j} \in \{\emptyset, \text{a common vertex, edge or face}\}$ for each $K_j, K_i \in \mathcal{T}_h$ (see [1]). Further, let us define a finite-dimensional space $X_h = \{v_h \in C(\overline{\Omega}) \mid v_h|_K \in P_1(K) \forall K \in \mathcal{T}_h\} \subset H^1(\Omega)$ and define also $V_h = X_h \cap V$.

If we denote $\{\varphi_h^m\}_{m=1}^{N_h}$ the basis of the space V_h and $u_{hDi}^k \in X_h$ the X_h -interpolation of \tilde{u}_{Di}^k , we can define the solution of (12)-(14) obtained by the finite elements method as $u_{hi}^k = u_{hDi}^k + \sum_{m=1}^{N_h} c_{i,m}^k \varphi_h^m$, where $c_{i,m}^k \in \mathbb{R}$, $i = 1, 2, \dots, N$. The function u_{hi}^k then satisfies

- $u_{hi}^{k+1} - u_{hDi}^{k+1} \in V_h$
- and for all $s = 1, 2, \dots, N_h$ holds

$$\sum_{m=1}^{N_h} b_{i,sm}^k c_{i,m}^{k+1} = f_{i,s}^k, \text{ where}$$

$$b_{i,sm}^k = \left(\frac{1}{\tau} - r_i\right)(\varphi_m, \varphi_s) + D_i(\nabla \varphi_m, \nabla \varphi_s) + \sum_{j=1}^N a_{ij}(u_j^k \varphi_m, \varphi_s) \quad \text{and} \quad (15)$$

$$f_{i,s}^k = \frac{1}{\tau}(u_{hi}^k, \varphi_s) + D_i(g_i^{k+1}, \varphi_s)_{\Gamma_N} - \left(\frac{1}{\tau} - r_i\right)(u_{hDi}^{k+1}, \varphi_s) - D_i(\nabla u_{hDi}^{k+1}, \nabla \varphi_s) - \sum_{j=1}^N a_{ij}(u_{hj}^k u_{hDi}^{k+1}, \varphi_s). \quad (16)$$

Thus one can compute a vector $\mathbf{c}_i^{k+1} = (c_{i,s}^{k+1})_{s=1}^{N_h}$ by solving the system of linear equations $\mathbb{B}_i^k \mathbf{c}_i^{k+1} = \mathbf{f}_i^k$ with a matrix $\mathbb{B}_i^k = (b_{i,sm}^k)_{s,m=1}^{N_h}$ and a right-hand side $\mathbf{f}_i^k = (f_{i,s}^k)_{s=1}^{N_h}$.

3.2 Mesh Adaptivity

When using some advanced techniques (e.g. [2]) for mesh-adaptation, we have to combine the properties of all N functions and thus it is necessary to construct one function that is a "combination" of them. This function should change its value rapidly wherever any of N functions changes its value rapidly. One can construct such a function for instance in a following way: At each node P_j of the triangulation \mathcal{T}_h let us order all values $u_{hi}^k(P_j)$, $i = 1, 2, \dots, N$, in such a way that $u_{hi_m}^k(P_j) \geq u_{hi_{m+1}}^k(P_j)$ for $m = 1, 2, \dots, N-1$. Then the value of the compound function ψ_h^k at P_j is defined by

$$\psi_h^k(P_j) = \sum_{m=1}^N (-1)^{m+1} u_{hi_m}^k(P_j). \quad (17)$$

However, one has to also choose a suitable projection between a new and the old mesh. This projection can reduce an order of convergence or even result in a nonconsistency of the method.

4 Error Analysis

While solving partial differential equations numerically, one has to estimate the error of applied numerical method. The required estimates are provided by the following theorem (see [3]).

Theorem 2. Let $\tau \in \left(0, \frac{1}{\rho + \|\mathbb{A}\|_\infty M}\right)$, where $\rho = \max_i r_i$, $M = \max_i M_i$ and $\|\mathbb{A}\|_\infty = \max_i \sum_{j=1}^N a_{ij}$. Further, let $u_i, u_i' \in L^\infty(0, T, H^{s+1}(\Omega))$, $u_i'' \in L^\infty(0, T, L^2(\Omega))$ and $g_i \in L^\infty(0, T, H^{s+1}(\Gamma_N))$ for each $i = 1, 2, \dots, N$, and any $s \geq 0$. Then there exist constants $C_L, C_H > 0$ independent from τ, h and $\beta = \max_i D_i$, such that

$$\|e_h\|_{\mathcal{S}, \infty}^2 = \max_{0 \leq k \leq p} \|e_h^k\|_{\mathcal{S}}^2 = \max_{\substack{0 \leq k \leq p \\ 0 \leq i \leq N}} \|e_{hi}^k\|_2^2 \leq C_L \left(\tau^2 + \beta h^{2s} + h^{2(s+1)} + \beta^2 h^{2(s+1)} \right),$$

$$|e_h|_{\mathcal{S}, 2}^2 = \max_{0 \leq i \leq N} \left(\tau D_i \sum_{k=0}^p |e_{hi}^k|_1^2 \right) \leq C_H \left(\tau^2 + \beta h^{2s} + h^{2(s+1)} + \beta^2 h^{2(s+1)} \right).$$

The Theorem rests upon division of the error into two parts. The estimate of the discretization error comes from the approximative properties of the finite element spaces. The error of the numerical method is estimated using Young's inequality and boundedness of \mathbf{u}_h and time derivatives of \mathbf{u} .

5 Numerical Results

5.1 Example 1 - Neumann Boundary Conditions

In $\Omega = [0, 1]^2$ we solve a problem (12)-(14) with $N = 3$, $\Gamma_D = \emptyset$ and coefficients $D_i = 10^{-4}$ and $r_i = 1$, for $i = 1, 2, 3$. In addition $a_{11} = a_{22} = a_{33} = 1$, $a_{12} = a_{23} = a_{31} = 2$ and $a_{21} = a_{13} = a_{32} = 7$. Initial conditions are chosen in such a way that $u_{0i} = \chi_{\mathcal{M}_i}$, for $i = 1, 2, 3$, where

$$\mathcal{M}_1 = \{(x, y) \in \Omega \mid (x - 0.23)^2 + (y - 0.2)^2 \leq (1/4)^2\}, \quad (18)$$

$$\mathcal{M}_2 = \{(x, y) \in \Omega \mid (x - 0.67)^2 + (y - 0.75)^2 \leq (1/5)^2\}, \quad (19)$$

$$\mathcal{M}_3 = \{(x, y) \in \Omega \mid (x - 0.75)^2 + (y - 0.5)^2 \leq (3/10)^2\}. \quad (20)$$

The invariant region of this problem is a block $[0, M_1] \times [0, M_2] \times [0, M_3]$, where $M_i = \max\{\|u_{0i}\|_\infty, 1\} = 1$ for $i = 1, 2, 3$. Further, we choose $T = 100$ with $p = 200$ and thus $\tau_k = 0.5$. Neumann boundary conditions are homogeneous, i.e. $g_i^k = 0$, for $i = 1, 2, 3$ and $k = 0, 1, \dots, p$. The interpolation of the initial condition and a solution computed at $T = 100$ are depicted on Figures 1 and 2.

5.2 Example 2 - Dirichlet Boundary Conditions

In $\Omega = [0, 1]^2$ we solve a problem (12)-(14) with $N = 3$, $\Gamma_N = \emptyset$ and coefficients $D_i = 10^{-4}$ and $r_i = 1$, for $i = 1, 2, 3$. In addition $a_{11} = a_{22} = a_{33} = 1$, $a_{12} = a_{23} = a_{31} = 2$ and $a_{21} = a_{13} = a_{32} = 7$. Initial conditions are chosen in such a way that $u_{0i} = \chi_{\mathcal{M}_i}$, for $i = 1, 2, 3$, where

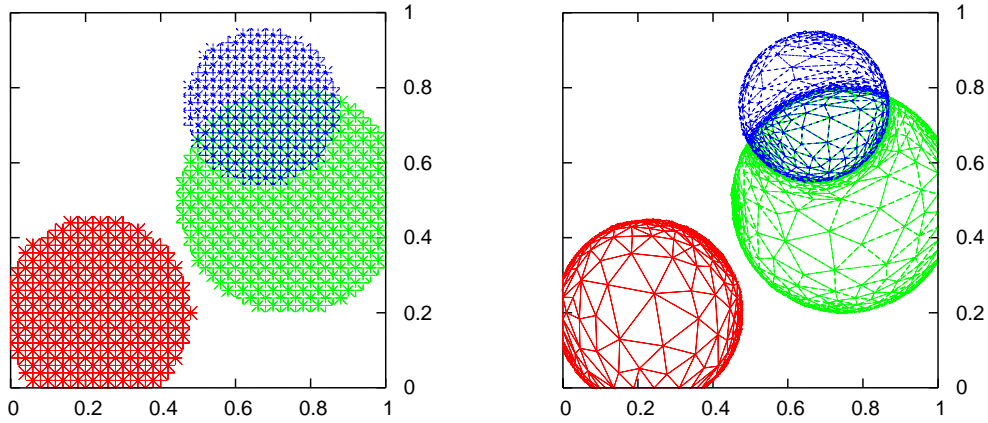
$$\mathcal{M}_1 = \{(x, y) \in \Omega \mid 9(x - 0.4)^2 + 25(y - 0.65)^2 \leq 1\}, \quad (21)$$

$$\mathcal{M}_2 = \{(x, y) \in \Omega \mid (x - 0.67)^2 + (y - 0.65)^2 \leq (1/5)^2\}, \quad (22)$$

$$\mathcal{M}_3 = \{(x, y) \in \Omega \mid (x - 0.6)^2 + (y - 0.4)^2 \leq (3/10)^2\}. \quad (23)$$

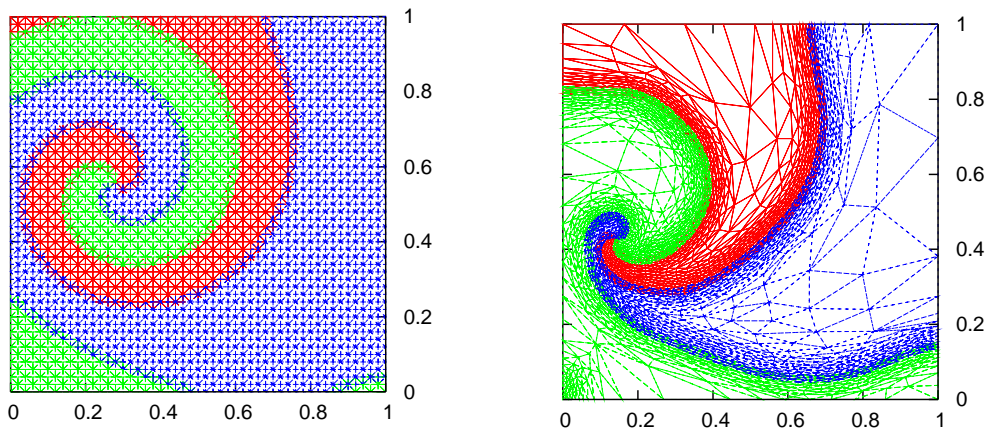
We choose $T = 50$ with $p = 100$ and thus $\tau_k = 0.5$. Dirichlet boundary conditions are $u_{Di}^k(x, y) = y$, for all $i = 1, 2, 3$ and $k = 0, 1, \dots, p$.

Since $\|u_{Di}^k\|_\infty = 1$, the invariant region of this problem is the same as the previous one. The interpolation of the initial condition and a solution computed at $T = 50$ are depicted on Figures 3 and 4.



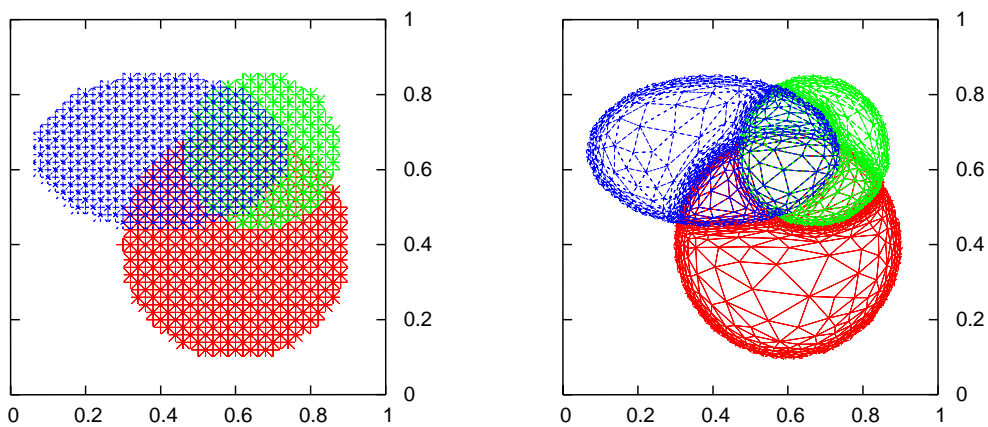
Source: Own

Fig. 1. The interpolation of the initial condition of Example 1 on an isotropic (left, 5000 elements, 2601 nodes) and adapted mesh (right, 2724 elements, 1301 nodes)



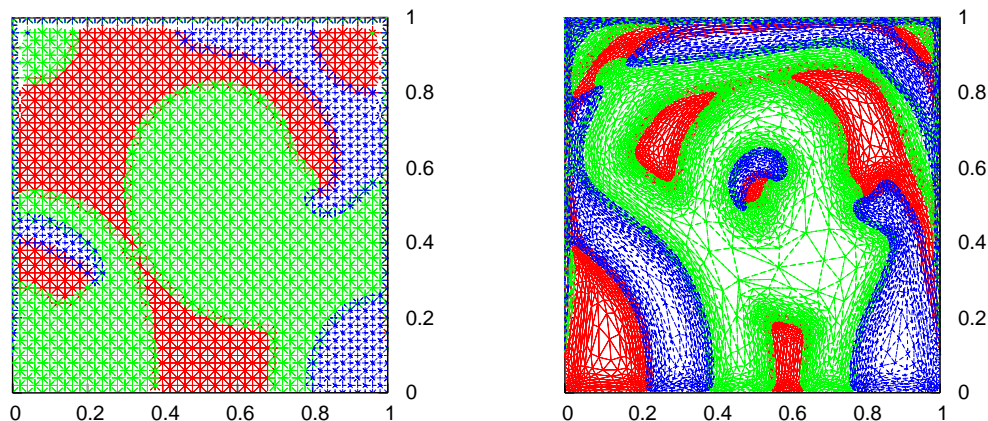
Source: Own

Fig. 2. The solution of Example 1 computed at $T = 100$ on an isotropic (left, 5000 elements, 2601 nodes) and adapted mesh (right, 3694 elements, 1899 nodes)



Source: Own

Fig. 3. The interpolation of the initial condition of Example 2 on an isotropic (left, 5000 elements, 2601 nodes) and adapted mesh (right, 1760 elements, 3501 nodes)



Source: Own

Fig. 4. The solution of Example 2 computed at $T = 50$ on an isotropic (left, 5000 elements, 2601 nodes) and adapted mesh (right, 5021 elements, 9830 nodes)

Conclusion

We have successfully derived and tested a numerical method for solving reaction-diffusion equations. We have also proven that for sufficiently smooth and suitable data the solution of the equations is continuous and belongs to the space $\mathcal{C}((0, T), L^2(\Omega))$. For numerical solution we have used the Galerkin finite elements method and derived a priori error estimates on isotropic meshes. We have used adaptively refined meshes as well, however, the error estimates are no longer valid on them. In order to obtain error estimates on adapted meshes a better projection should be used.

Acknowledgments

This work was supported by the European Social Fund project for constitution and improvement of a team for demanding technical computations on parallel computers at Technical University of Liberec, reg. num. CZ.1.07/2.3.00/09.0155, the research programme num. MSM6840770010, by the research center of Ministry of Education, Youth and Sports num. LC06052 and by the Grant Agency of the Czech Republic, grant No. P201/11/1304.

Literature

- [1] CIARLET, P. G.: *The finite element method for elliptic problems*. North-Holland Publishing Company, Amsterdam-New York-Oxford, 1978.
- [2] DOLEJŠÍ, V.: ANGENER, version 3.1 - Fortran source package able to generate triangulations [online]. Available from WWW: <<http://www.karlin.mff.cuni.cz/~dolejsi/angen/angen3.1.htm>>
- [3] DOLEJŠÍ, V.; FEISTAUER, M.: Analysis of semiimplicit DGFEM for nonlinear convection-diffusion problems. *Preprint Series of the School of Mathematics*, Charles University Prague, No. MATH-KNM-2004/1, 2004.
- [4] ESLEROVÁ, L.: *Numerická analýza dynamiky reakčně-difuzních rovnic*. Master's Thesis, Department of mathematics FJFI ČVUT, 1996.

- [5] HOLODNIOK, M. et al.: *Metody analýzy nelineárních dynamických modelů*. Academia, Praha, 1986.
- [6] LAMAČ, J.: *Numerické metody pro řešení reakčně-difuzních rovnic*. Rešeršní práce, Department of mathematics FJFI ČVUT, Praha, 2009.
- [7] LAMAČ, J.: *Numerické metody pro řešení reakčně-difuzních rovnic*. Výzkumný úkol, Department of mathematics FJFI ČVUT, Praha, 2010.
- [8] LAMAČ, J.: *Numerické metody pro řešení reakčně-difuzních rovnic*. Master's Thesis, Department of mathematics FJFI ČVUT, Praha, 2012.
- [9] REKTORYS, K.: *The method of discretization in time and partial differential equations*. SNTL-Publishers, Praha, 1985.
- [10] SMOLLER, J.: *Shock Waves and Reaction-Diffusion Equations*. Springer Verlag, New York - Heidelberg - Berlin, 1983.

NUMERICKÉ ŘEŠENÍ REAKČNĚ-DIFUZNÍCH ROVNIC

Obsahem předložené práce je matematická analýza a numerické řešení soustavy nelineárních nestacionárních difuzně-reakčních rovnic. Nejprve je s využitím invariantního regionu proveden důkaz existence a jednoznačnosti řešení a spojitě závislosti na datech úlohy. Po časové diskretizaci problému je aplikována Galerkinova metoda konečných prvků a odvozeny apriorní odhady chyby numerické metody. Rovněž je diskutována vhodná adaptace použitých triangulací. Na závěr je celá metoda implementována a otestována na různých příkladech.

NUMERISCHE LÖSUNG REAKTIONSDIFFUSER GLEICHUNGEN

Der Inhalt der vorgelegten Arbeit besteht in der mathematischen Analyse und der numerischen Lösung des Systems nichtlinearer nicht stationärer reaktionsdiffuser Gleichungen. Zunächst wird unter Verwendung einer invarianten Region der Beweis der Existenz und der Eindeutigkeit der Lösung und der kontinuierlichen Abhängigkeit von den Daten der Aufgabe erbracht. Nach einer zeitlichen Diskretisierung des Problems wird die Galerkin-Methode der finiten Elemente angewandt und es werden A-priori-Schätzungen des Fehlers der numerischen Methode abgeleitet. Ebenfalls wird eine geeignete Adaption der gebrauchten Triangulationen diskutiert. Zum Abschluss wird die gesamte Methode implementiert und an verschiedenen Beispielen getestet.

NUMERYCZNE ROZWIĄZYWANIE RÓWNAŃ REAKCYJNO-DYFUZYJNYCH

Przedmiotem niniejszego opracowania jest analiza matematyczna oraz numeryczne rozwiązanie układu nieliniowych równań niestacjonarnych dyfuzyjno-reakcyjnych. W pierwszej kolejności przy wykorzystaniu niezmiennego regionu przeprowadzono dowód na istnienie i jednoznaczność rozwiązania oraz ciągłą zależność od danych zadania. Po czasowej dyskretyzacji problemu zastosowano metodę Galerkin elementów skończonych oraz oszacowano a priori błąd metody numerycznej. Omówiono także odpowiednią adaptację zastosowanych triangulacji. W zakończeniu przedstawiono zastosowanie całej metody i sprawdzono ją na różnych przykładach.