Kragujevac J. Math. 30 (2007) 151–170.

IMMERSED INTERFACE METHOD FOR A SYSTEM OF LINEAR REACTION-DIFFUSION EQUATIONS WITH NONLINEAR SINGULAR OWN SOURCES

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(Received November 9, 2006)

Dedicated to Professor Bosko S. Jovanović on the occasion of his 60th birthday

Abstract. A system of linear reaction-diffusion equations with nonlinear singular own sources is considered in this paper. Compatibility conditions provided sufficient regularity of the solution are derived. A second order accurate immersed interface difference scheme is constructed for the differential system of equations involving interfaces. The numerical method is more accurate than the standard approach and does not require the interfaces to be grid points. An algorithm for decoupling of the difference equations in nonlinear part (with small number of equations) and linear part (with large number of equations) is proposed. Numerical experiments are discussed.

1. INTRODUCTION

Many physical, biological, chemical and other problems lead to mathematical models in which the input data (such as the coefficients of the differential equations, initial conditions, source terms etc.) are discontinuous or even singular across one or several interfaces in the solution domain. These problems are called interface problems and their solutions typically are non-smooth or discontinuous across the interfaces.

Interface problems have attracted a lot of attention from both theoretical and numerical point of view. Many numerical methods designed for smooth solutions do not work for such problems. The standard discrete methods require the grid points to lie along the interfaces. Another methods use Cartesian grid and avoid grid regeneration. Some commonly used methods for discontinuous coefficients problems are the smoothing method that utilizes the smoothed Heaviside function, and harmonic averaging method. Similar is the Steklov operator method developed in the papers of Jovanovic, Vulkov [5, 6, 7].

Recently some new methods are developed to deal with interfaces with more complicated geometry. Most of them are motivated by the Peskin's immersed boundary method [16], originally constructed for studying the blood flow in the heart. It uses grid-dependent discrete Dirac δ functions to distribute singular source to nearby grid points and is first order of accuracy method. It was extended by Beyer and LeVeque [1], were the combination of different discrete δ functions gives second order results, but only for 1-D problems. In 1994 LeVeque and Li [9] developed the immersed interface method (IIM) for elliptic equations. Later, it has been extended to many others problems, see the review paper of Li [11].

The key idea of IIM is to incorporate the known jump conditions of a solution and its derivatives into finite difference schemes in the neighborhood of the discontinuities arising from the singular force. In [10] immersed interface finite element method is presented for the case of homogeneous jump conditions. Cartesian grids are used and then associated uniform triangulations are added on. Interfaces are not necessarily aligned with cell boundaries. Using modified bases functions it is second order method in maximum norm. In [23] an explicit jump immersed interface method for elliptic problems is developed. It uses the jump conditions of higher order to decrease the local truncation error of the finite difference schemes.

In this paper we consider another kind of conjugation conditions, see (5),(6), which are specific and are not treated in the papers mentioned above. The solution is continuous, but the jump of the flux depends on the solution at the active sites. One of the difficulties appeared is the wider stencil to make IIM work. For the one-dimensional case it needs 6-points on every time layer, while it needs 8-points for the two-dimensional problems with line interface, parallel to one of the axis [13]. Some classical difference schemes for the scalar case (S=1) of the problem (1)–(3) and single (R=1) site of reactions are examined in [3]. The IIM for one equation (S=1) and many reactions is studied in [13] and for the parabolic system (1)–(3) with one reaction (S=1) - in [22]. 2-D parabolic problems with more complicated interfaces are considered in [14]. Boundary element approximations of (1)–(3) are derived in [17].

We propose a fast numerical method, which combines a second order IIM difference scheme and an algorithm for solving the discrete equations. The layout of the paper is as follows. The differential problem is stated in the next section. Existence and uniqueness of regular solution of the problem formulated is also discussed. The IIM difference scheme is derived in Section 3. An algorithm based on elimination of the unknowns corresponding to linear equations is presented in Section 4. It essentially decreases the computational work. Finally, numerical experiments are discussed in the last section.

2. THE DIFFERENTIAL PROBLEM

In this paper we construct and analyze an IIM difference scheme for the system of reaction-diffusion equations

$$\frac{\partial U}{\partial t} = D\frac{\partial^2 U}{\partial x^2} - \Omega U + \sum_{r=1}^{R} Q_r(U)\delta(x-\xi_r) \tag{1}$$

$$(x,t) \in Q_T = \Omega \times (0,T),\ \Omega = (-1,1),\ 0 < t < T,$$

$$U(x,0) = U_0(x), \quad \text{for } x \in \Omega, \tag{2}$$

and

$$U(-1,t) = \Phi(t),\ U(1,t) = \Psi(t), \quad 0 < t < T. \tag{3}$$

Here $U(x,t) = (u_1(x,t), ..., u_S(x,t))^T$ is a vector of concentration of S different species, $D = diag(D_1, ..., D_S)$ is a diagonal matrix of diffusion coefficients, $\Omega = (w_{ij}),\ i,j = 1, ..., S$ is a matrix corresponding to adsorption-desorption linear processes and $Q_r(U) = (Q_{1r}(U), ..., Q_{Sr}(U))^T$ is the r-th reaction term due to reaction taking place at active site $\xi_r, r = 1, ..., R$.

These equations describe various physical processes with localized source terms. For example, localized reactions occur at chemically active parallel line deflects on a two-dimensional surface. Similar phenomena are also observed in biological systems, for instance on chemically active membranes. The reader can consult [2, 17] for physical derivation.

The additional motivation for our study comes from the parabolic problems with interfaces. In [4] the authors study the well-posedness of a scalar diffusion equation of the above type. Sufficient conditions are found to ensure global existence and blow-up time. There are not such results for the system (1) in the literature. On the other hand an effective numerical approach to (1)–(3) will help at studying of the qualitative behaviour of the solutions.

With some assumptions for smoothness a solution of (1)–(3) is equivalent to a solution of the following problem:

$$\frac{\partial U}{\partial t} = D\frac{\partial^2 U}{\partial x^2} - \Omega U, x \in (-1,1), x \neq \xi_r, 0 < t < T, \tag{4}$$

$$[U]_{\xi_r} \equiv U(\xi_r + 0, t) - U(\xi_r - 0, t) = 0,\ 0 \leq t \leq T,\ r = 1, ..., R, \tag{5}$$

$$D[\frac{\partial U}{\partial x}]_{\xi_r} = -Q_r(U(\xi_r, t)),\ 0 \leq t \leq T,\ r = 1, ..., R, \tag{6}$$

subjected with initial (2) and boundary conditions (3).

This is a parabolic problem and if the input data are piecewise functions, the solution is also piecewise function. The discontinuities of the solution and its derivatives propagates along the discontinuity lines $x = \xi_r,\ r = 1, ..., R$.

For construction of a second-order accurate IIM difference scheme that approximates (4)-(6), (2), (3) we need some regularity of the solution $U(x,t)$. Let $C^0_\alpha = C_\alpha$ be the set of the Holder continuous functions with $0 < \alpha < 1$. For each $k \geq 1$ we introduce the following subspaces $C^k_\alpha(Q_T)$ of $C_\alpha(Q_T)$, whose elements have Holder continuous derivatives:

$$C^k_\alpha(Q_T) = \{u : \frac{\partial^{i+j} u}{\partial x^i \partial t^j} \in C^0_\alpha(Q_T), \quad 0 \le i + 2j \le k, \quad \text{i,j - nonnegative integers}\}.$$

In order the solution U to be continuous up to the boundary $\{(x,t) : x = -1, +1, 0 \le t \le T\}$ and up to the interface $\Gamma_T = \{(x,t) : x = \xi_r, \ r = 1, ..., R, \ 0 \le t \le T\}$ it is necessary to have the following conditions:

$$u_{s,0}(-1) = \varphi_s(0), \ u_{s,0} = \psi_s(0), \ [u_{s,0}]_{\xi_r} = 0, \ s = 1, ..., S, \ r = 1, ..., R.$$

We call these relations *compatibility conditions of order 0.*

If we require the solution to have continuous derivatives $\partial U/\partial t$, $\partial^2 U/\partial x^2$ up to the boundary the following conditions are necessary:

$$\dot\varphi_s(0) = u''_{s,0}(-1), \ \ \dot\psi_s(0) = u''_{s,0}(1), \ \text{ where } \ s = 1, ..., S, \ \cdot \equiv d/dt, \ \ ' \equiv d/dx.$$

Differentiating the equality (5) with respect to t we get

$$\left[\frac{\partial u_s}{\partial t}\right]_{\xi_r} = 0, \ s = 1, ..., S, \ r = 1, ..., R. \tag{7}$$

Now, from (4),(5) and (7), one obtains

$$D_s \left[\frac{\partial^2 u_s}{\partial x^2}\right]_{\xi_r} = 0, \ s = 1, ..., S, \ r = 1, ..., R. \tag{8}$$

Therefore,

$$D_s \left[u''_{s,0}\right]_{\xi_r} = 0, \ s = 1, ..., S, \ r = 1, ..., R. \tag{9}$$

Also, it follows from (8), that

$$D_s \left[u'_{s,0}\right]_{\xi_r} = -Q_{sr}(U_0(\xi_r)), \ s = 1, ..., S, \ r = 1, ..., R. \tag{10}$$

Conditions (16), (17) are called *compatibility conditions of order 1.*

Next, differentiating (4) with respect to x we find

$$\left[\frac{\partial^2 u_s}{\partial t \partial x}\right]_{\xi_r} = D_s \left[\frac{\partial^3 u_s}{\partial x^3}\right]_{\xi_r} - \sum_{i=1}^{S} \omega_{si} \left[\frac{\partial u_i}{\partial x}\right], \ s = 1, ..., S, \ r = 1, ..., R. \tag{11}$$

Differentiating the equality (6) with respect to t we find expressions for $[\partial^2 u_s/\partial t\partial x]_{\xi_r}$, $s=1,...,S,\ r=1,...,R$. With this, (11) becomes:

$$\left[\frac{\partial^3 u_s}{\partial x^3}\right]_{\xi_r} = -\frac{1}{D_s}\sum_{i=1}^{S}\left(\frac{1}{D_s}\frac{\partial Q_{sr}}{\partial u_i}\frac{\partial u_i}{\partial t} + \omega_{si}Q_{ir}\right)_{\xi_r} \quad s=1,...,S,\ r=1,...,R. \qquad (12)$$

Now, from (4), (7) and (12) it follows the *compatibility conditions of order 2*:

$$\left[u'''_{s,0}\right]_{\xi_r} = -\frac{1}{D_s}\sum_{i=1}^{S}\left(\frac{1}{D_s}\frac{\partial Q_{sr}}{\partial u_i}\left(D_i u''_{i,0}(\xi_r) - \sum_{s=1}^{S}\omega_{is}u_{s,0}(\xi_r)\right) + \omega_{si}Q_{ir}\left(U_0(\xi_r)\right)\right),$$
$$s=1,...,S,\ r=1,...,R.$$

It was found that the compatibility conditions are not only necessary for the continuity of the corresponding derivatives of U up to the boundary and the interface, they are also sufficient. The following result for local existence and uniqueness of solution holds [4, 8, 18].

Theorem 1. *Let* $U_0 \in C_\alpha[-1,1] \cap C^2_\alpha(-1,0) \cap C^2_\alpha(0,1)$ *has continuous derivatives,* $\varphi,\ \psi \in C^1_\alpha[0,T]$ *and* $Q(u) \in C^1(R^S)$. *Assume that the compatibility conditions of order* 0 *and* 1 *are hold. Then the problem (1)-(3) has a unique solution* $u \in C_\alpha(\bar{Q}_T)$ $\cap\ C^2_\alpha(Q_T\backslash\Gamma_T)$ *and this solution also solves the problem (4)-(6), (2), (3).*

If the compatibility conditions of order 2 *are also hold, then* $u \in C_\alpha(\bar{Q}_T) \cap C^3_\alpha(Q_T\backslash\Gamma_T)$.

3. CONSTRUCTION OF AN IIM DIFFERENCE SCHEME

We discretize (1)-(3) on the mesh $\bar{\omega} = \bar{\omega}_h \times \bar{\omega}_\tau$:

$$\begin{aligned}\bar{\omega}_h &= \{x_i = ih\ ,\quad i=0,1,...,M,\quad x_0=-1,\quad x_M=1\},\\ \bar{\omega}_\tau &= \{t_{n+1} = t_n + \tau_{n+1}\ ,\quad n=0,1,...,N-1,\quad t_0=0,\quad t_N=T\}.\end{aligned}$$

Let denote the solution matrix as $U(t) = (U_1, U_2, \cdots, U_M)^T$, where $U_i = U(x_i,t)$. Define also $U^n = (U^n_1, U^n_2, \cdots, U^n_M)^T$, where $U^n_i = U(x_i,t_n)$.Our finite difference method described below produces the matrix $Y(t) = (Y_0(t), ..., Y_M(t))^T$, $0 < t < T$, that approximates $U(t)$ and $Y^n = (Y_0^n, ..., Y_M^n)^T$ for $n = 0, ..., N$, that approximates U^n (superscript T denotes transpose). For simplicity, we may also write $\check{Y}_i = Y_i^n$, $\hat{Y}_i = Y_i^{n+1}$, $i = 0, ..., M$, $n = 0, ..., N-1$.

On the mesh $\bar{\omega}_h \times \bar{\omega}_\tau$ we shall use the standard notations, as in [20],

$$f_{\bar{x}}(x_i) = f_{\bar{x},i} = (f_i - f_{i-1})/h, \; f_x(x_i) = f_{x,i} = (f_{i+1} - f_i)/h,$$
$$f_{\bar{x}x}(x_i) = f_{\bar{x}x,i} = (f_x)_{\bar{x},i} \; .$$

Let us fix the integer r, $1 \le r \le R$ and suppose that $x_{I_r} \le \xi_r < x_{I_r+1}$, $2 \le I_r \le M-2$. The vector function $U(x,t)$ is smooth almost everywhere, except at ξ_r, $r = 1, ..., R$, where its derivatives has a discontinuity of first kind. Therefore, the question is how to approximate the derivatives $\partial^2 u_s(x_{I_r}, t)/\partial x^2$, $\partial^2 u_s(x_{I_r+1}, t)/\partial x^2$, $s = 1, ..., S$, $r = 1, ..., R$ using the solution values at grid points. From the Taylor expansion, we obtain a second order difference at a grid point x_j, $j = I_r, I_{r+1}$, as did in [1]:

$$\begin{aligned} \frac{\partial^2 u_s(x_j,t)}{\partial x^2} &= u_{s,\bar{x}x}(x_j,t) \\ - \quad & \frac{sgn(\xi_r - x_j)}{h^2} \sum_{m=0}^{\infty} \frac{1}{m!} \left(h^2 sgn(\xi_r - x_j) d_h^{(1)}(x_j - \xi_r)\right)^m \left[\frac{\partial^m u_s}{\partial x^m}\right]_{\xi_r}, \end{aligned} \tag{13}$$

where $d_h^{(1)}$ is the Peskin's discrete delta function, or "hat function" with support $(-h, h)$:

$$d_h^{(1)}(x) = \begin{cases} (h - |x|)/h^2, & |x| \le h, \\ 0, & otherwise. \end{cases}$$

It follows from (13) that to achieve second order accuracy, the solution $u_s(x,t)$, $s = 1, ..., S$, must have up to third order piecewise continuous derivatives. The discontinuity occurs at the interface Γ_T. The compatibility conditions require that the initial data $u_{s,0}(x)$, $s = 1, ..., S$ and the reaction terms f_r, $r = 1, ..., R$ also to have second order piecewise continuous derivatives.

Plugging (6), (8), (12) for $[\partial^m u_s/\partial x^m]_{\xi_r}$, $m = 1, 2, 3$, $s = 1, ..., S$, $r = 1, ..., R$ into (20), we obtain the desired second order approximation. Now, the equations (4)–(6) can be written in the form:

$$\frac{\partial u_s(x_i,t)}{\partial t} = D_s u_{s,\bar{x}x}(x_i,t) - \sum_{k=1}^{S} \omega_{sk} u_k(x_i,t) + 0(h^2) \tag{14}$$
$$i = 1,...,M-1,\ i \neq I_r, I_r+1,\ s = 1,...,S,\ r = 1,...,R,$$

$$\begin{aligned}\frac{\partial u_s(x_{I_r},t)}{\partial t} &= D_s u_{s,\bar{x}x}(x_{I_r},t) - \sum_{k=1}^{S} \omega_{sk} u_k(x_{I_r},t) + \frac{x_{I_r+1}-\xi_r}{h^2} Q_{sr}(U(\xi_r,t)) \\ &+ \frac{(x_{I_r+1}-\xi_r)^3}{6h^2} \tilde{Q}_{sr}(U(\xi_r,t)) + 0(h^2),\end{aligned} \tag{15}$$

$$\begin{aligned}\frac{\partial u_s(x_{I_r+1},t)}{\partial x^2} &= D_s u_{s,\bar{x}x}(x_{I_r+1},t) - \sum_{k=1}^{S} \omega_{sk} u_k(x_{I_r+1},t) - \frac{x_{I_r}-\xi_r}{h^2} Q_{sr}(U(\xi_r,t)) \\ &- \frac{(x_{I_r}-\xi_r)^3}{6h^2} \tilde{Q}_{sr}(U(\xi_r,t)) + 0(h^2),\end{aligned} \tag{16}$$

where

$$\tilde{Q}_{sr}(U(\xi_r,t)) = \sum_{k=1}^{S} \left(\frac{1}{D_s} \frac{\partial Q_{sr}}{\partial u_k} \frac{\partial u_k}{\partial t} + \omega_{sk} Q_{kr} \right)_{\xi_r},\ s = 1,...,S,\ r = 1,...,R.$$

Since in the IIM ξ_r usually does not coincide with any of the nodes x_{I_r}, x_{I_r+1}, we need to interpolate $u_s(\xi_r,t)$ and $\partial u_s(\xi_r,t)/\partial t$. We use the interpolation formula from Lemma 4.2 in [1]:

$$\varphi(\xi_r) = h \sum_j \varphi(x_j) d_h(x_j - \xi_r) + 0(h^p). \tag{17}$$

Here φ is an arbitrary continuous function, Lipschitz continuous on each half interval,

$$\varphi \in C^{p-1}\left([\xi_r - Lh, \xi_r) \cup (\xi_r, \xi_r + Lh]\right), \tag{18}$$

and $d_h(x)$ satisfies:

$$d_h(x) = 0 \text{ for } |x| \geq Lh,\ L - \text{integer};$$
$$h \sum_j (x_j - \xi_r)^m d_h(x_j - \xi_r) = \delta_{m0} = \begin{cases} 1, & m = 0, \\ 0, & m = 1,...,p-1. \end{cases} \tag{19}$$

To preserve $0(h^2)$ approximation in (15), (16) we apply (17) to $\partial u_s(\xi_r,t)/\partial t$ and $u_s(\xi_r,t)$. For this we need $d_h^{(1)}$ and the following discrete delta-function:

$$d_h^{(6)}(x) = \frac{1}{2h} \begin{cases} (h-|x|)(h+|x|)(2h+|x|)/h^3, & |x| \leq h, \\ 2(h-|x|)(h+|x|)(2h-|x|)/h^3, & h \leq |x| \leq 2h, \\ (h-|x|)(2h-|x|)(3h-|x|)/h^3, & 2h \leq |x| \leq 3h, \\ 0, & otherwise. \end{cases}$$

The condition (18) with $d_h^{(6)}$ applied to $u(\xi_r, t)$ requires the following restriction on the mesh size:

$$3h < \min_{1\le i\le R+1}(\xi_i - \xi_{i-1}), \tag{20}$$

where $\xi_0 = x_0,\ \xi_{R+1} = x_M$.

To approximate $Q_{sr}(U(\xi_r, t))$ and $\partial Q_{sr}(U(\xi_r, t))/\partial u_k,\ s, k = 1, ..., S,\ r = 1, ..., R$, we apply the so called "product approximation formula" [19]:

$$\begin{aligned}
\frac{\partial Q_{sr}(U(\xi_r,t))}{\partial u_k} &= \frac{\partial Q_{sr}\left(h\sum_j U(x_j,t)d_h^{(1)}(x_j-\xi_r)+O(h)\right)}{\partial u_k}\\
&= h\sum_j \frac{\partial Q_{sr}(U(x_j,t))}{\partial u_k}d_h^{(1)}(x_j-\xi_r)+O(h)\\
&\approx \rho_{I_r+1}\frac{\partial Q_{sr}(U(x_{I_r},t))}{\partial u_k}+\rho_{I_r}\frac{\partial Q_{sr}(U(x_{I_r+1},t))}{\partial u_k},
\end{aligned}$$

$$\begin{aligned}
Q_{sr}(U(\xi_r,t)) &= Q_{sr}\left(h\sum_j U(x_j,t)d_h^{(6)}(x_j-\xi_r)+0(h^3)\right)\\
&= h\sum_j Q_{sr}(U(x_j,t))d_h^{(6)}(x_j-\xi_r)+0(h^3)\\
&\approx \theta_{1r}Q_{sr}(U(x_{I_r-2},t))+\theta_{2r}Q_{sr}(U(x_{I_r-1},t))+\theta_{3r}Q_{sr}(U(x_{I_r},t))\\
&+ \theta_{4r}Q_{sr}(U(x_{I_r+1},t))+\theta_{5r}Q_{sr}(U(x_{I_r+2},t))+\theta_{6r}Q_{sr}(U(x_{I_r+3},t))\\
&= \sum_{i=1}^{6}\theta_{ir}Q_{sr}(U(x_{I_r-3+i},t)) \equiv \overline{\overline{Q}}_{sr},
\end{aligned}$$

where for $r = 1, ..., R$

$$\begin{aligned}
\rho_{I_r} &= (\xi_r - x_{I_r})/h, & \rho_{I_r+1} &= (x_{I_r+1}-\xi_r)/h,\\
\theta_{1r} &= \rho_{I_r}\rho_{I_r+1}(\rho_{I_r}+1)/2, & \theta_{2r} &= -\rho_{I_r}\rho_{I_r+1}(\rho_{I_r}+2),\\
\theta_{3r} &= \rho_{I_r+1}(\rho_{I_r}+1)(\rho_{I_r}+2)/2, & \theta_{4r} &= \rho_{I_r}(\rho_{I_r+1}+1)(\rho_{I_r+1}+2)/2,\\
\theta_{5r} &= -\rho_{I_r}\rho_{I_r+1}(\rho_{I_r+1}+2), & \theta_{6r} &= \rho_{I_r}\rho_{I_r+1}(\rho_{I_r+1}+1)/2.
\end{aligned}$$

Now, we neglect high order terms of $O(h^2)$ in (14)-(16) to get the following semi-discrete problem:

$$
\begin{aligned}
(E-\rho_{I_r+1}d_rD^{-1}\overline{Q}'_r)\dot{Y}_{I_r} \quad &- \quad \rho_{I_r}d_rD^{-1}\overline{Q}'_r\dot{Y}_{I_r+1}\\
&= \Phi_{r,1}(Y_{I_r-2},Y_{I_r-1},Y_{I_r},Y_{I_r+1},Y_{I_r+2},Y_{I_r+3})\\
&= DY_{\bar{x}x,I_r}-\Omega Y_{I_r}+e_r\overline{\overline{Q}}_r+d_r\Omega D^{-1}\overline{Q}_r, \qquad (21)
\end{aligned}
$$

$$
\begin{aligned}
-\rho_{I_r+1}m_rD^{-1}\overline{Q}'_r\dot{Y}_{I_r} \quad &+ \quad (E-\rho_{I_r}m_rD^{-1}\overline{Q}'_r)\dot{Y}_{I_r+1}\\
&= \Phi_{r,1}(Y_{I_r-2},Y_{I_r-1},Y_{I_r},Y_{I_r+1},Y_{I_r+2},Y_{I_r+3})\\
&= DY_{\bar{x}x,I_r+1}-\Omega Y_{I_r+1}+g_r\overline{\overline{Q}}_r+m_r\Omega D^{-1}\overline{Q}_r, \qquad (22)
\end{aligned}
$$

$$
\dot{Y}_i = DY_{\bar{x}x,i}-\Omega Y_i, \quad i=1,...,M-1, \quad i\neq I_r, I_r+1\ , \quad r=1,...,R, \qquad (23)
$$

where E is the identity matrix of size S,

$$
\begin{aligned}
d_r &= \frac{h}{6}\rho^3_{I_r+1}, \quad e_r=\frac{\rho_{I_r+1}}{h}, \quad m_r=\frac{h}{6}\rho^3_{I_r}, \quad g_r=\frac{\rho_{I_r}}{h},\\
\overline{Q}_r &= \rho_{I_r+1}Q_r(Y_{I_r})+\rho_{I_r}Q_r(Y_{I_r+1})\\
\overline{\overline{Q}}_r &= \sum_{i=1}^{6}\theta_{ri}Q_r(Y_{I_r-3+i})\\
\overline{Q}'_r &= \rho_{I_r+1}Q'_r(Y_{I_r})+\rho_{I_r}Q'_r(Y_{I_r+1})\\
Q'_r &= \begin{pmatrix} \partial Q_{1r}/\partial u_1 \dots \partial Q_{1r}/\partial u_S\\ \vdots \\ \partial Q_{Sr}/\partial u_1 \dots \partial Q_{Sr}/\partial u_S \end{pmatrix}. \qquad (24)
\end{aligned}
$$

Let denote

$$
A_r(Y_{I_r},Y_{I_r+1}) = \left\| \begin{matrix} A_{r,11} & A_{r,12}\\ A_{r,21} & A_{r,22}\end{matrix} \right\| = \left\| \begin{matrix} E-\rho_{I_r+1}d_rD^{-1}\overline{Q}'_r & -\rho_{I_r}d_rD^{-1}\overline{Q}'_r\\ -\rho_{I_r+1}d_rD^{-1}\overline{Q}'_r & E-\rho_{I_r}d_rD^{-1}\overline{Q}'_r\end{matrix} \right\|. \qquad (25)
$$

The inverse matrix A^{-1} is

$$
A_r^{-1}(Y_{I_r},Y_{I_r+1}) = \left\| \begin{matrix} P_{r,11} & P_{r,12}\\ P_{r,21} & P_{r,22}\end{matrix} \right\|,
$$

where

$$
\begin{aligned}
P_{r,22} &= (A_{r,22}-A_{r,21}A^{-1}_{r,11}A_{r,12})^{-1}, \qquad & P_{r,12} &= -A^{-1}_{r,11}A_{r,12}P_{r,22},\\
P_{r,21} &= -P_{r,22}A_{r,21}A^{-1}_{r,11}, & P_{r,11} &= -A^{-1}_{r,11}-A^{-1}_{r,11}A_{r,12}P_{r,21}.
\end{aligned}
$$

Then we find the explicit form of the unknowns $\dot{Y}_{I_r}$, $\dot{Y}_{I_r+1}$, $r = 1, ..., R$:

$$\begin{aligned} \dot{Y}_{I_r} &= P_{r,11}\Phi_{r,1} + P_{r,12}\Phi_{r,2}, \\ \dot{Y}_{I_r+1} &= P_{r,21}\Phi_{r,1} + P_{r,22}\Phi_{r,2}. \end{aligned}$$

The semi-discretization (21)–(23) is an intermediate step in the derivation of a fully discrete scheme. In this paper, we apply the semi-implicit Euler's method (with weight $0 \le \sigma \le 1$) to obtain the system of finite difference equations between time level t^n and t^{n+1}:

$$\hat{Y}_0 = F_0 = 0, \quad \hat{Y}_M = F_M = 0, \tag{26}$$

$$-A_i\hat{Y}_{i-1} + C_i\hat{Y}_i - B_i\hat{Y}_{i+1} = F_i, \quad i = 1, ..., M-1,\ i \ne I_r, I_r+1,\ r = 1, ..., R, \tag{27}$$

$$\hat{Y}_{I_r} - \tau\sigma(P_{r,11}\hat{\Phi}_{r,1} + P_{r,12}\hat{\Phi}_{r,2}) = \tau(1-\sigma)(P_{r,11}\check{\Phi}_{r,1} + P_{r,12}\check{\Phi}_{r,2}) - \check{Y}_{I_r}, \tag{28}$$

$$\hat{Y}_{I_r+1} - \tau\sigma(P_{r,21}\hat{\Phi}_{r,1} + P_{r,22}\hat{\Phi}_{r,2}) = \tau(1-\sigma)(P_{r,21}\check{\Phi}_{r,1} + P_{r,22}\check{\Phi}_{r,2}) - \check{Y}_{I_r+1}, \tag{29}$$

where

$$A_i = (\tau\sigma/h^2)E, \quad B_i = A_i, \quad C_i = E + 2A_i + \tau\Omega, \quad F_i = \check{Y}_i + \tau(1-\sigma)\check{Y}_{\bar{x}x,i}.$$

It is obvious that the local truncation error of the weighted scheme (26)–(29) is of $O(\tau^m + h^2)$, where $m = 1$ if $\sigma \ne 0.5$ and $m = 2$ if $\sigma = 0.5$.

4. ALGORITHM FOR DECOUPLING OF THE NONLINEAR EQUATIONS

A three stage algorithm for solving the system (26)–(29) is proposed below:

- *first*, we eliminate all unknown vectors except $\hat{Y}_{I_r}$, $\hat{Y}_{I_r+1}$, $r = 1, ..., R$;
- *second*, we solve $\hat{Y}_{I_r}$ and $\hat{Y}_{I_r+1}$, $r = 1, ..., R$ using an iteration method for the system of $2R$ nonlinear equations;
- *third*, find other unknown vectors using the exact recurrent formulas.

We seek the mesh solution in the form

$$\hat{Y}_i = Z_i + \sum_{r=1}^{R}(V_i^{I_r}\hat{Y}_{I_r} + V_i^{I_r+1}\hat{Y}_{I_r+1}), \quad i = 0, ..., M, \tag{30}$$

where Z_i is a vector with S components and $V_i^{I_r}$, $V_i^{I_r+1}$ are matrixes of order S.

It follows from this linear form:

$$Z_0 = F_0,\ Z_M = F_M,\ Z_{I_r} = 0,\ Z_{I_r+1} = 0,\ r = 1, ..., R;$$

$$V_0^{I_r} = V_M^{I_r} = V_0^{I_r+1} = V_M^{I_r+1} = 0;$$

$$V_i^{I_r} = \begin{cases} E,\ i = I_r, & r = 1, ..., R, \\ 0,\ i = I_r + 1,\ I_k, I_k + 1,\ k \neq r,\ k = 1, ..., R; \end{cases}$$

$$V_i^{I_r+1} = \begin{cases} E,\ i = I_r + 1, & r = 1, ..., R, \\ 0,\ i = I_r,\ I_k, I_k + 1,\ k \neq r,\ k = 1, ..., R. \end{cases}$$

Plugging the relations (30) into (27), we get a linear system of equations for three groups of unknowns $\{Z_i\}$, $\{V_i^{I_r}\}$, $\{V_i^{I_r+1}\}$. The unknowns $\{Z_i\}$ are found from the systems:

$$Z_0 = F_0,$$

$$-A_i Z_{i-1} + C_i Z_i - B_i Z_{i+1} = F_i,\ i = 1, ..., I_1 - 1,$$

$$Z_{I_1} = 0;$$

$$\begin{gathered} Z_{I_k+1} = 0\ , \\ -A_i Z_{i-1} + C_i Z_i - B_i Z_{i+1} = F_i,\ i = I_k + 2, ..., I_{k+1} - 1,\ k = 1, ..., R - 1, \\ Z_{I_{k+1}} = 0; \end{gathered} \tag{31}$$

$$Z_{I_R+1} = 0,$$

$$-A_i Z_{i-1} + C_i Z_i - B_i Z_{i+1} = F_i,\ i = I_R + 2, ...,\ M - 1,$$

$$Z_M = F_M.$$

We set $I_0 = -1,\ I_{R+1} = M$. In order to find $\{V_i^{I_k}\},\ i = 1, ..., M - 1,\ k = 1, ..., R$, we solve the following linear systems with $k = 1, ..., R$ and $r = 1, ..., R + 1$,

$$\begin{gathered} V_{I_{r-1}+1}^{I_k} = 0,\ V_{I_r}^{I_k} = \begin{cases} 0\ ,\ k \neq r, \\ E\ ,\ k = r, \end{cases} \\ -A_i V_{i-1}^{I_k} + C_i V_i^{I_k} - B_i V_{i+1}^{I_k} = 0,\ i = I_{r-1} + 2, ...,\ I_r - 1. \end{gathered} \tag{32}$$

In a similar way can be determined the unknowns $\{V_i^{I_k+1}\}$: for $k = 1, ..., R$ and $r = 1, ..., R+1$ we solve the linear systems

$$V_{I_r}^{I_k+1} = 0 \ , \ V_{I_{r-1}+1}^{I_k+1} = \begin{cases} 0 \ , \ k \neq r-1, \\ E \ , \ k = r-1, \end{cases} \tag{33}$$
$$-A_i V_{i-1}^{I_k+1} + C_i V_i^{I_k+1} - B_i V_{i+1}^{I_k+1} = 0 \ , \ i = I_{r-1}+2, ..., I_r - 1.$$

Now, from (30), we get the expression for $\hat{Y}_{I_r-2}$, $\hat{Y}_{I_r-1}$, $\hat{Y}_{I_r+2}$, $\hat{Y}_{I_r+3}$:

$$\begin{aligned} \hat{Y}_{I_r-2} &= Z_{I_r-2} + V_{I_r-2}^{I_{r-1}+1}\hat{Y}_{I_{r-1}+1} + V_{I_r-2}^{I_r}\hat{Y}_{I_r}, \\ \hat{Y}_{I_r-1} &= Z_{I_r-1} + V_{I_r-1}^{I_{r-1}+1}\hat{Y}_{I_{r-1}+1} + V_{I_r-1}^{I_r}\hat{Y}_{I_r}, \\ \hat{Y}_{I_r+2} &= Z_{I_r+2} + V_{I_r+2}^{I_r+1}\hat{Y}_{I_r+1} + V_{I_r+2}^{I_{r+1}}\hat{Y}_{I_{r+1}}, \\ \hat{Y}_{I_r+3} &= Z_{I_r+3} + V_{I_r+3}^{I_r+1}\hat{Y}_{I_r+1} + V_{I_r+3}^{I_{r+1}}\hat{Y}_{I_{r+1}}. \end{aligned} \tag{34}$$

Inserting (34) in (28)–(29) we get a nonlinear system of $2R$ equations:

$$\begin{aligned} G_{r1}(\hat{Y}_{I_{r-1}+1}, \hat{Y}_{I_r}, \hat{Y}_{I_r+1}, \hat{Y}_{I_{r+1}}) = \hat{Y}_{I_r} - \tau\sigma(\hat{\tilde{P}}_{r,11}\hat{\tilde{\Phi}}_{r,1} + \hat{\tilde{P}}_{r,12}\hat{\tilde{\Phi}}_{r,2}) \\ -\tau(1-\sigma)(\check{\tilde{P}}_{r,11}\check{\tilde{\Phi}}_{r,1} + \check{\tilde{P}}_{r,12}\check{\tilde{\Phi}}_{r,2}) - \check{Y}_{I_r} = 0, \end{aligned} \tag{35}$$

$$\begin{aligned} G_{r2}(\hat{Y}_{I_{r-1}+1}, \hat{Y}_{I_r}, \hat{Y}_{I_r+1}, \hat{Y}_{I_{r+1}}) = \hat{Y}_{I_r+1} - \tau\sigma(\hat{\tilde{P}}_{r,21}\hat{\tilde{\Phi}}_{r,1} + \hat{\tilde{P}}_{r,22}\hat{\tilde{\Phi}}_{r,2}) \\ -\tau(1-\sigma)(\check{\tilde{P}}_{r,21}\check{\tilde{\Phi}}_{r,1} + \check{\tilde{P}}_{r,22}\check{\tilde{\Phi}}_{r,2}) - \check{Y}_{I_r+1} = 0 \end{aligned} \tag{36}$$

where $\tilde{P}_{r,kl}$ and $\tilde{\Phi}_{r,k}$, $\ r = 1, ..., R, \ k, l = 1, 2$ are obtained from $P_{r,kl}, \ \Phi_{r,k}$ after the substitution. Note that for $r = 1$, we have $Y_{I_{r-1}+1} = Y_0$ and for $r = R$ we have $Y_{I_{R+1}} = Y_M$.

The most widely used iterative method for solving the nonlinear algebraic system of equations, obtained from the finite difference discretization, is the Newton's method, see for example [15]. We apply the classical Newton's method to (35), (36). For shorter we rewrite the system in the form:

$$G_{r1} = \hat{Y}_{I_r} - \tau\sigma\hat{H}_{r,1} - \tau(1-\sigma)\check{H}_{r,2} - \check{Y}_{I_r} = 0, \tag{37}$$

$$G_{r2} = \hat{Y}_{I_r+1} - \tau\sigma\hat{H}_{r,2} - \tau(1-\sigma)\check{H}_{r,2} - \check{Y}_{I_r+1} = 0. \tag{38}$$

Let us denote the incremental $\delta Y_i \equiv \delta Y_i^{j+1} = \delta \overset{s+1}{Y}_i = \overset{s+1}{Y}_i - \overset{s}{Y}_i$, $i = I_r, I_{r+1},\ r = 2, ..., R-1$, where $\overset{s}{Y}_i$ is the approximate value of $\hat{Y}_i$ at the s-th iteration. Then the $(s+1)$-th iteration can be written as follows:

$$-\tau L_{2r-1,2r-2}\delta Y_{I_{r-1}+1} + (E - \tau L_{2r-1,2r-1})\delta Y_{I_r}$$
$$-\tau L_{2r-1,2r}\delta Y_{I_r+1} - \tau L_{2r-1,2r+1}\delta Y_{I_{r+1}} = -\overset{s}{G}_{r1} \tag{39}$$

$$-\tau L_{2r,2r-2}\delta Y_{I_{r-1}+1} - \tau L_{2r,2r-1}\delta Y_{I_r}$$
$$+(E - \tau L_{2r,2r})\delta Y_{I_r+1} - \tau L_{2r,2r+1}\delta Y_{I_{r+1}} = -\overset{s}{G}_{r2}, \tag{40}$$

where for $r = 1, ..., R$

$$L_{i,j} = \frac{\partial H_{r,k}}{\partial Y_j},\quad i = 2r + k - 2,\quad j = 2r - 2,\ 2r - 1,\ 2r,\ 2r + 1,\ k = 1, 2 \tag{41}$$

is the Jacobian matrix of the vector function H_{rk} by the components of the vector Y_j.

This linear system of algebraic equations has a special form and we propose the following factorization algorithm, which is a variant of Thomas-type algorithm [21]:

- *Forward substitution*:

$$\beta_0^2 = 0,\ \gamma_0^2 = \delta Y_0 = 0,$$

$$\alpha_r^1 = \tau\sigma D_{r1}^{-1} L_{2r-1,2r},\quad \beta_r^1 = \tau\sigma D_{r1}^{-1} L_{2r-1,2r},$$

$$\gamma_r^1 = D_{r1}^{-1}(\overset{s}{G}_{r1} + \tau\sigma L_{2r-1,2r-2}\gamma_{r-1}^2),$$

$$\beta_r^2 = D_{r2}^{-1}(D_{r3}\beta_r^1 - \tau\sigma L_{2r,2r+1}),$$

$$\gamma_r^2 = D_{r2}^{-1}(-\overset{s}{G}_{r2} + \tau\sigma L_{2r,2r-2}\gamma_{r-1}^2 - D_{r3}\gamma_r^1),$$

  where for $r = 1, ..., R$

$$D_{r1} = E - \tau\sigma(L_{2r-1,2r-2}\beta_{r-1}^2 + L_{2r-1,2r-1}),$$

$$D_{r2} = D_{r1}\alpha_r^1 + E - \tau\sigma L_{2r,2r},\quad D_{r3} = -\tau\sigma(L_{2r,2r-2}\beta_{r-1}^2 + L_{2r,2r-1}).$$

- *Backward substitution*:

$$\delta Y_{I_{R+1}} = \delta Y_M = 0,$$

and for $r = R, ..., 1$

$$\delta Y_{I_r+1} = \beta_r^2 \delta Y_{I_{r+1}} + \gamma_r^2, \quad \delta Y_{I_r} = \alpha_r^1 \delta Y_{I_r+1} + \beta_r^1 \delta Y_{I_{r+1}} + \gamma_r^1.$$

Therefore, given an initial data one could advance from n-th ($n = 0, ..., N-1$) time layer to the next one by the algorithm just described. This algorithm will converge, if D_{r1} and D_{r2} are not singular matrix. A more careful analysis similar to those in [13] gives us the following theorem.

Theorem 2. *Suppose that the functions $Q_r(U)$ have continuous derivatives up to third order on a every bounded interval $I \subset \mathbf{R}^1$. If the solution of the finite difference equation $\check{Y}(\check{Y}_1, ..., \check{Y}_M)$ at n-th time layer satisfies*

$$C_{Q_U}(\check{Y}) \equiv \max_{1\le r\le R}(\max(|Q_U(\check{Y}_{I_r})|, |Q_U(\check{Y}_{I_r+1})|)) < \frac{3}{h}, \tag{42}$$

then for sufficiently small τ there exists unique solution of the system (37), (38). Newton's method applied to the non-linear system of equations with initial approximation $Y^0 = \check{Y}$ converges quadratically.

5. NUMERICAL EXPERIMENTS

Example 1. We start with a system of two equations ($S = 2$) and single active site ($R = 1$) at which nonlinear reactions occur. On the domain $Q_T = \{(x, t) : x \in (0, 2), t \in (0, T]\}$ we consider the following problem:

$$\frac{\partial u_1}{\partial t} = D_1 \frac{\partial^2 u_1}{\partial x^2} + Q_1(u_1, u_2)\delta(x - \xi),$$
$$\frac{\partial u_2}{\partial t} = D_2 \frac{\partial^2 u_2}{\partial x^2} + Q_2(u_1, u_2)\delta(x - \xi),$$

with initial and zero boundary conditions

$$u_1(x, 0) = u_2(x, 0) = 1 - |1 - x|, \;\; x \in (0, 2),$$
$$u_1(-1, t) = u_1(1, t) = u_2(-1, t) = u_2(1, t) = 0, \;\; t \in .$$

In this problem we choose $\xi = 1$ and a reaction terms $Q = (Q_1, Q_2)$ associated with the Lotka-Volterra system of ordinary differential equations:

$$Q_1(u_1, u_2) = 4u_1 - 4u_1u_2,$$
$$Q_2(u_1, u_2) = -4u_2 + 4u_1u_2.$$

The problem has two equilibrium study state solutions $(0, 0)$ and $(1.5, 0.5)$. It is known that the solution (0,0) is not stable and the second one is stable.

In Fig. 1 we present the phase diagram of the solutions (u_1, u_2) at the active site $\xi = 1$ at final time $T = 5$, $N = 64$, and $M = 2000$. As it seen for this initial and boundary conditions the numerical solution goes to the stable solution $(1.5, 0.5)$. We chose the parameter T to be $T = 5$ and $T = 50$. We have no a closed form solution, so in the numerical experiments we compare the computed solution at final time T with the study state solution. In Table 1 we present the error in maximum norm $error_1 = |y_1(1, T) - 1.5|$ and the rate of convergency m. Mesh refinement analysis confirms second order of accuracy of the method. Other results are discussed in [22].

Table 1: Mesh refinement analysis in maximum norm for the *Example 1.*

$T = 5$				$T = 50$			
M	N	$error_1$	m	M	N	$error_1$	m
32	400	1.4995e-02	-	32	1000	9.8543e-02	-
64	800	3.1748e-03	2.26	64	2000	3.0921e-02	1.67
128	1600	7.1371e-04	2.12	128	4000	9.3516e-03	1.73
256	3200	1.8564e-04	1.95	256	8000	2.5017e-03	1.90
512	6400	4.6748e-05	1.98	512	16000	5.9282e-04	2.07

Example 2. We consider a system of two equations ($S = 2$) and two active sites ($R = 2$) at which nonlinear reactions occur. On the domain $Q_T = \{(x, t) : x \in (0, 2), t \in (0, T]\}$ we state the problem:

$$\frac{\partial u_1}{\partial t} = D_1 \frac{\partial^2 u_1}{\partial x^2} + Q_{11}(u_1, u_2)\delta(x - \xi_1) + Q_{12}(u_1, u_2)\delta(x - \xi_2),$$
$$\frac{\partial u_2}{\partial t} = D_2 \frac{\partial^2 u_2}{\partial x^2} + Q_{21}(u_1, u_2)\delta(x - \xi_1) + Q_{22}(u_1, u_2)\delta(x - \xi_2),$$

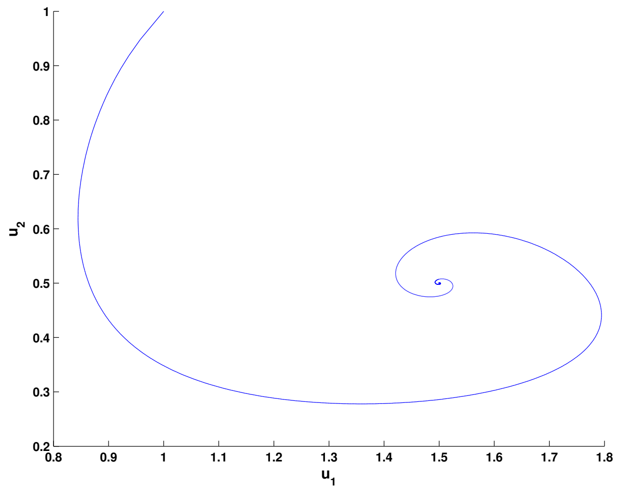

Figure 1: Phase diagram of the solution (u_1, u_2) at the active site $x = \xi = 1$ for *Example 1* at final time $T = 5$, $N = 64$, and $M = 2000$.

with initial and zero boundary conditions

$$u_1(x,0) = u_2(x,0) = 1 - |1-x|, \ x \in (0,2),$$
$$u_1(-1,t) = u_1(1,t) = u_2(-1,t) = u_2(1,t) = 0, \ t \in (0,T].$$

In this problem we choose $\xi_1 = 1$, $\xi_2 = 1.5$ and the reaction terms (Q_{11}, Q_{21}), (Q_{21}, Q_{22}) to be

$$Q_{11}(u_1,u_2) = 4u_1 - 4u_1u_2,$$
$$Q_{12}(u_1,u_2) = -4u_2 + 4u_1u_2.$$

$$Q_{21}(u_1,u_2) = 4u_1 + 4u_1u_2,$$
$$Q_{22}(u_1,u_2) = 4u_2 + 4u_1u_2.$$

In Fig. 2 we present the evolution of the solution u_1 on the left and u_2 on the right. The signs and the nonlinearity of the reaction terms at the active site ξ_2 lead to the blow up solutions for u_1 and u_2. It confirms the theoretical results in [4]. If the reaction terms at the active site ξ_2 are chosen similar to those at ξ_1

$$Q_{21}(u_1,u_2) = 4u_1 - 4u_1u_2,$$
$$Q_{22}(u_1,u_2) = -4u_2 + 4u_1u_2,$$

then no blow up solutions occur.

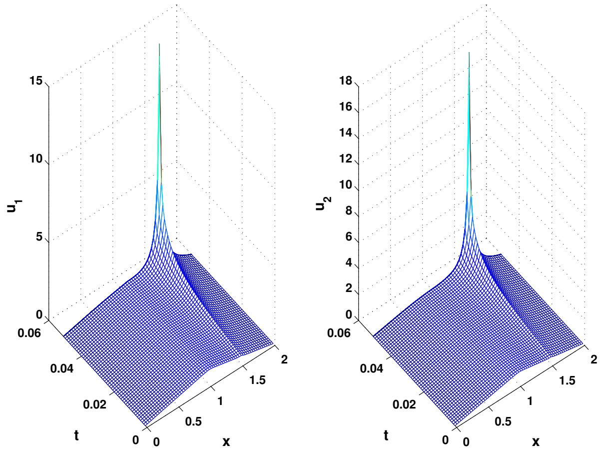

Figure 2: Evolution of u_1 on the left and u_2 on the right for *Example 2* at final time $T = 0.5112$, $N = 64$, and $\tau = 10^{-5}$.

Acknowledgements: This work was supported by the National Science Fund of Bulgaria under contract HS-MI-106/2005.

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