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THE NUMERICAL SOLUTION OF NON-LINEAR PSEUDO-PARABOLIC EQUATIONS

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Abstract. This paper is devoted to numerical methods for mathematical modelling a quasi-stationary process in semiconductors. New effective methods are offered for non-classical PDE with non-linear and non-local coefficients.

Key words: pseudo-parabolic equations, semiconductors, non-linear equations, Rosenbrock schemes

1. Introduction

In 1953 S.L. Sobolev [7] had attracted attention to mathematical problems of dynamics of rotated liquid and had given a strict deduction of the equation describing small oscillations of such liquid

$$\Delta u_{tt} + \alpha^2 u_{x_3 x_3} = 0. \tag{1.1}$$

Then scientists have paid attention to the fact that some other physical processes were described by equations which were very similar to the equation (1.1), for example waves in stratified liquid, ion-acoustic waves in non-magnetized plasma, waves in transmission lines. Usually equations of Sobolev type result from reduction of vector system of PDEs to one scalar high order equation [4, 5].

Thus mathematical model of wave processes in such media is initial boundary value problem for one scalar high order PDE. The investigations of such problems are carried out by numerical and analytical methods. Analytical methods allow proving theorems of existence and uniqueness of solution, getting double-ended estimations for the life time of solution, obtaining conditions of global existence of solutions for any time [3]. But it is possible to obtain explicit solutions by analytical methods only for very special and simple problems. Numerical methods allow investigating solution in details. Therefore we shall consider general numerical methods.

2. Numerical Methods for Pseudo-Parabolic Equations

From the point of view of numerical methods it is useful to select three types of equations. The first type equations include linear operators under derivative by time:

$$(\Delta u - u)_t + e^u = 0. \tag{2.1}$$

The second type equations include non-linear operators under derivative by time:

$$\left(\Delta u - u^3\right)_t + \Delta u + u^5 = 0. \tag{2.2}$$

The third type equations include non-local coefficients depending on a norm of the solution:

$$(\Delta u - u)_t + \|u\|_2^p \, \Delta u = 0. \tag{2.3}$$

The combination of second and third type equations is also possible.

For numerical solution of initial-boundary value problems for these equations we use the method of lines. All differential operators on spatial variables are approximated by finite-differences. So the PDE is reduced to a system of ODE of large dimension. For numerical solution of this system it is very important to use integration methods which are suitable for stiff problems. Among such methods we pay attention to two methods: implicit Runge-Kutta method and Rosenbrock method.

For some of investigated equations the conditions of solution collapse are known. Destruction of solution corresponds to a breakdown in semiconductor. Numerical experiments on embedded meshes allowed us to determine the exact moment of breakdown and to diagnose the singularity type.

3. Rosenbrock Method

The main advantage of Rosenbrock method is that nonlinear systems do not arise. In case of autonomous system $u_t = F(u)$ the one stage Rosenbrock looks as follows [6]:

$$\hat{u}_n = u_n + \tau \mathrm{Re} k_n, \quad (E - \alpha \tau F_u)\, k_n = F(u_n)\,.$$

Depending on a complex valued parameter α this scheme has various properties. If $\alpha = (1+i)/2$ then scheme has second order of accuracy and it is L_2 stable. This scheme is called CROS. In case of implicit systems $M u_t = F(u)$ this scheme looks as follows

$$\hat{u}_n = u_n + \tau \mathrm{Re} k_n, \quad (M - \alpha \tau F_u)\, k_n = F(u_n)\,. \tag{3.1}$$

Moreover M may be a singular matrix. In this case the system becomes a differential algebraic system [2]. There is only one restriction: matrix M can not depend on u or t.

4. Tests on Embedded Grids

Let p be theoretical order of accuracy of the discrete solution. If we carry out calculations on two different grids with numbers of points N and rN, then estimation of the error is given by the Richardson formula

$$\Delta^{(rN)}(t) = \frac{u^{(rN)}(t) - u^{(N)}(t)}{r^p - 1} + o\left(N^{-p}\right). \tag{4.1}$$

It is possible to get the effective order of accuracy by using discrete solutions on three grids with numbers of points N, rN, r^2N:

$$p^{eff}(t) = \log_r \frac{u^{(rN)}(t) - u^{(N)}(t)}{u^{(r^2N)}(t) - u^{(rN)}(t)}. \tag{4.2}$$

If $p^{eff}(t) \to p$, then solution is smooth enough and the error estimation by the Richardson formula is asymptotically exact. This approach allows us to determine the moment of solution destruction. When a solution is not smooth the difference between p^{eff} and p^{theor} becomes large. From significance of p^{eff} it is possible to make a conclusion about the type of singularity [1].

5. Numerical Results

We shortly described methods and approaches, which we use in our work. Now let's consider concrete examples. First we define equations with linear operator under derivative by time

$$\begin{cases} (u_{xx} - u)_t + e^u = 0, \\ u|_{t=0} = u_0(x), \quad u|_{x=0} = u|_{l=0} = 0. \end{cases} \tag{5.1}$$

For the indicated initial-boundary value problem some theoretical results are known. In particular existence of classical solution was proved and the double-ended estimations for life time of solution were obtained. By approximating the differential operator on uniform spatial grid we get the system of implicit ordinary differential equations $Mu_t = F(u)$ with 3-diagonal matrix M. The CROS scheme was used for solving this problem.

It is convenient to illustrate the technique of determination the time of solution destruction with the help of tables, in which the significance of the effective order of accuracy are indicated at different instants and different points of the segment. As it was already marked above the effective order of accuracy tends to theoretical if number of knots tends to infinity. Therefore small deviation from $p^{eff} \approx 2$ does not testify yet destruction of solution.

However at t= 0.34 the discontinuous modification of effective order happens at once in all view points. And we can determine time of destruction with error about length of a time step.

As it was marked above there are double-ended estimations for the life time of solution which depends on initial data. We decided to calculate these

Table 1. Effective order of accuracy at different time moments

t	0.26	0.52	0.79	1.05	1.31	1.57	1.83	2.09	2.36	2.62	2.88
0,04	2.00	2.00	2.00	2,01	2.00	2.00	2.00	2,01	2.00	2.00	2.008
0,16	2.00	2.00	1,99	1,97	2,01	2,01	2,01	1,97	1,99	2.00	2.00
0,28	1,99	1,99	1,98	1,98	1,98	1,97	1,98	1,98	1,98	1,99	1,99
0,32	1,95	1,95	1,95	1,95	1,95	1,95	1,95	1,95	1,95	1,95	1,95
0,34	**1,36**	**1,36**	**1,37**	**1,41**	**1,56**	**1,71**	**1,56**	**1,41**	**1,37**	**1,36**	**1,36**
0,36	**0,06**	**0,06**	**0,09**	**0,27**	**1,01**	**2,17**	**1,01**	**0,27**	**0,09**	**0,06**	**0,06**

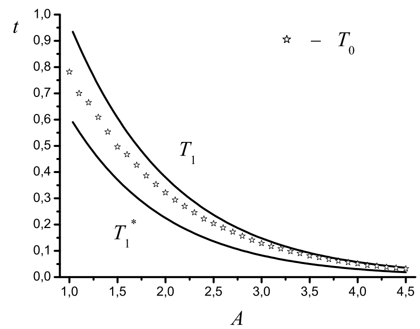

Figure 1. Double-ended estimation of breakdown moment T_-, T_+ in semiconductors and experimental value T.

estimations for different initial data $u_0(x) = A \sin x$ and compare them with significance obtained from the tests on embedded grids. Fig. 1 illustrates these calculations.

Let us consider the second type of equation

$$\left(u_{xx} - u - u^3\right)_t + u_{xx} + u(u+1)(u-2) = 0.$$

If we apply the method of lines to this equation then we get an implicit system of ODE, where matrix M depends on u and we can not use the Rosenbrock scheme. Therefore we will use a different approach. Introducing function $W = u_{xx} - u - u^3$ we obtain the following system:

$$\begin{cases} W_t + u_{xx} + u(u+1)(u-2) = 0, \\ W - \left(u_{xx} - u - u^3\right) = 0. \end{cases}$$

Using the method of lines we get the following differential algebraic system with singular matrix M

$$M \frac{d}{dt} \begin{pmatrix} W \\ U \end{pmatrix} = F \begin{pmatrix} W \\ U \end{pmatrix}, \quad M = \begin{pmatrix} E & 0 \\ 0 & 0 \end{pmatrix}.$$

This matrix does not depend on U, W and t so it is possible to use the Rosenbrock scheme. The problem of disintegration of rectangular impulse was solved. Depending on initial data two regimes are possible: either the solution tends to a stationary limit or it collapses in bounded time (see Fig. 2).

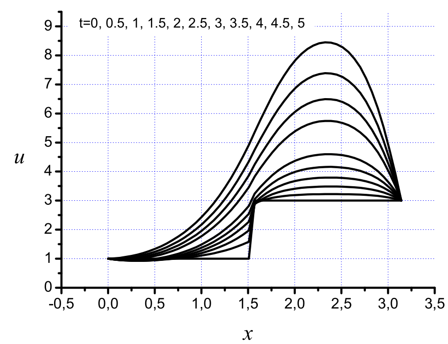

Figure 2. Numerical solution profiles for solution blow-up.

The next example describes the following initial boundary value problem:

$$\begin{cases} \left(u_{xx} - |u|^{q_1} u\right)_t + u_{xx} + |u|^{q_2} u = 0, \\ u|_{x=0} = u|_{x=l} = 0, \quad u|_{t=0} = u_0(x). \end{cases}$$

Here the behaviour of a solution essentially depends on parameters. If $q_2 < q_1$ then solution exists for any time. If $q_1 > q_2$ then solution exists for any time only for small initial data. If these sufficient conditions are not valid there is a collapse of the solution in bounded time

$$\|u_0\|_{q_2+2}^{q_2+2} > \tfrac{q_2+2}{2} \|\nabla u_0\|_2^2,$$

$$\|u_0\|_{q_2+2}^{q_2+2} > \|\nabla u_0\|_2^2 + \frac{2\sqrt{2}q_2(q_1+2)^{1/2}}{q_2-q_1}\left[\tfrac{1}{2}\|\nabla u_0\|_2^2 + \tfrac{q_1+1}{q_2+2}\|u_0\|_2^2\right].$$

Introducing $w = u_{xx} - |u|^{q_1} u$ we get the system:

$$\begin{cases} \dfrac{\partial}{\partial t} W + u_{xx} + |u|^{q_2} u = 0, \\ w - \left(u_{xx} - |u|^{q_1} u\right) = 0. \end{cases}$$

Using the method of lines we obtain a differential algebraic system with singular matrix. Fig. 3 illustrates results of calculations.

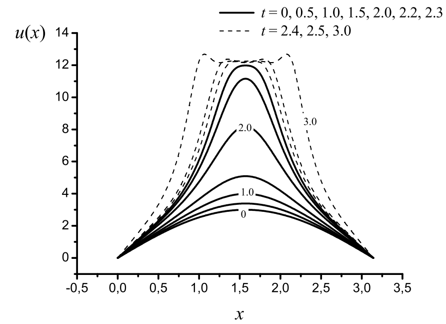

Figure 3. Profiles of numerical solution with singularity of logarithmic type.

6. Conclusions

The application of SMOL in combination with Rosenbrock scheme to the solution of pseudo-parabolic equations is rather effective. The non-local equations and equations with the nonlinear operator are necessary to be reduced to differential-algebraic systems with a constant matrix. The method of embedded grids allows to determine the moment and the type of solution singularity.

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