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CRANK-NICHOLSON DIFFERENCE SCHEMES FOR SOLVING COUPLED SYSTEMS OF NONLINEAR DIFFUSION EQUATIONS

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Abstract

It is shown how the set of nonlinear equations resulting from a Crank-Nicholson discretization of a system of nonlinear diffusion equations can be solved by Newton's iterative method.

It is proved: a) that the first step of this method is just a matter of solving a linearized (Crank-Nicholson) form of the diffusion equations, and b) that, under rather mild conditions, the matrices involved at each iteration are not singular.

1. INTRODUCTION

This report is concerned with numerical schemes for solving systems of nonlinear diffusion equations, which feature in many physical processes. For two functions u (r,t) and v (r,t) in a cylindrically symmetric configuration, for example, one obtains initial boundary value problems of the following type:

$$\frac{\partial u}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\phi^{(1)}\frac{\partial u}{\partial r} + r\phi^{(2)}\frac{\partial v}{\partial r}\right]$$

$$\frac{\partial v}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left[r\phi^{(3)}\frac{\partial u}{\partial r} + r\phi^{(4)}\frac{\partial v}{\partial r}\right] \tag{1}$$

$$u(r,0) = u_A(r) \geqq 0 \;,\; v(r,0) = v_A(r) \geqq 0 \text{ for } 0 \leqq r \leqq R \tag{1a}$$

$$u(R,t) = u_R(t) \geqq 0 \;,\; v(R,t) = v_R(t) \geqq 0 \text{ for } 0 \leqq t \leqq T \tag{1b}$$

$$\frac{\partial u(0,t)}{\partial r} = \frac{\partial v(0,t)}{\partial r} = 0 \quad \text{for} \quad 0 \leqq t \leqq T \tag{1c}$$

Here R is the cylinder radius, and T the length of time for which the diffusion process is considered. The regularity condition (1c) derives direct from cylindrical symmetry. Moreover, it is assumed that

$$\phi^{(i)} = \phi^{(i)}(u,v,\partial u/\partial r,\ \partial v/\partial r) \;,\quad i = 1,2,3,4 \tag{2}$$

as concerns the functional dependence of the diffusion coefficients $\phi^{(i)}$ both on the solutions, u, v and on their space derivatives (fluxes) $\partial u/\partial r$, $\partial v/\partial r$.

Finally, the system considered in this report contains just two equations, but the method discussed can be applied to systems of any number of equations. The linearized Crank-Nicholson method already proposed by D. Düchs some years ago has proved to be highly successful in treating such problems by means of difference schemes (see [1], [2], [3]). It is just a matter of solving a system of linear equations at each time step, without any loss of consistency compared with the complete nonlinear difference approximation, i.e. the order of the truncation error in the step sizes Δr, Δt is 2 in both methods. Furthermore, convergence of the linearized scheme was proved in 1979 (see [3]), by imposing certain conditions on the diffusion coefficients (2). Apart from these advantages, however, choosing large time steps Δt produces more or less strong oscillations in the solution curves. While it is true that Crank-Nicholson schemes are subject to such oscillations when the ratio of Δt to Δr becomes large, the following question nevertheless arises:

Is the maximum permissible size of time step, from the physical point of view, already exceeded whenever such a large (i.e. oscillation generating) time step Δt is chosen or are these "poor" solutions due to the linearization (which may perhaps suppress essential quantities)?

This question of great practical importance is treated in this report. It is shown that the linearized scheme turns out to be nothing but an iteration step of the multi-dimensional Newton method for solving the complete system of nonlinear difference equations. Systematic numerical experiments to be illustrated in a future report [4] show a surprising improvement on the linearized scheme when two or more Newton iterations are performed. This provides a definite answer to the question asked above, for a large class of examples at least:

The "poor" solutions with large step sizes Δt are primarily due to the linearization. The maximum Δt physically permissible obviously exceeds (to an appreciable extent in some cases) the maximum Δt that can be handled for linearization. Besides the advantages of the Newton method (very fast convergence, good results even when there are strong nonlinearities), there are also disadvantages: Firstly, the derivatives of the nonlinear functions resulting from the difference equations have to be calculated and the values in the functional matrix have to be recalculated for every Newton iteration. Secondly, the Newton method is known to be only locally convergent. It is therefore obvious that other standard methods of solving systems of nonlinear equations have to be enlisted for comparison (a comparison with the predictor-corrector method is therefore made in the second part of the forthcoming report.)

2. DIFFERENCE APPROXIMATIONS

To abbreviate the initial boundary value problem (1), the following notations are introduced:

$$W: = \begin{pmatrix} U \\ \\ \\ V \end{pmatrix}, \quad \phi: = \begin{pmatrix} \phi^{(1)} & \phi^{(2)} \\ & \\ & \\ \phi^{(3)} & \phi^{(4)} \end{pmatrix}, \quad W_A: = \begin{pmatrix} U_A \\ \\ \\ V_A \end{pmatrix}, \quad W_R: = \begin{pmatrix} U_R \\ \\ \\ V_R \end{pmatrix}$$

Equations (1) can then be written in the form

$$\frac{\partial W}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left[r\phi \left(W, \frac{\partial W}{\partial r}\right) \frac{\partial W}{\partial r} \right] \tag{1*}$$

$$W(r,0) = W_A(r) \geqq 0 \qquad \text{for} \quad 0 \leqq r \leqq R \tag{1*a}$$

$$W(R,t) = W_R(t) \geqq 0 \qquad \text{for} \quad 0 \leqq t \leqq T \tag{1*b}$$

$$\frac{\partial W}{\partial r} (0,t) = 0 \qquad \text{for} \quad 0 \leqq t \leqq T \tag{1*c}$$

The elements of the matrix function ϕ depend on four variables. Let the partial derivative of the function $\phi^{(\mu)}$ with respect to the ν - th variable be denoted by $D_\nu \phi^{(\mu)}$ $(\nu,\mu = 1, \ldots 4)$. We now define the following tensors:

$$D_1\phi \; : = \left\{ \begin{pmatrix} D_1\phi^{(1)} & D_1\phi^{(2)} \\ D_1\phi^{(3)} & D_1\phi^{(4)} \end{pmatrix}, \begin{pmatrix} D_2\phi^{(1)} & D_2\phi^{(2)} \\ D_2\phi^{(3)} & D_2\phi^{(4)} \end{pmatrix} \right\}$$

$$D_2\phi \; : = \left\{ \begin{pmatrix} D_3\phi^{(1)} & D_3\phi^{(2)} \\ D_3\phi^{(3)} & D_3\phi^{(4)} \end{pmatrix}, \begin{pmatrix} D_4\phi^{(1)} & D_4\phi^{(2)} \\ D_4\phi^{(3)} & D_4\phi^{(4)} \end{pmatrix} \right\}$$

Furthermore, we express products of these tensors by means of two-component vectors $x = (x_1, x_2)^T$ as follows:

$$D_1\phi\cdot x: = \left\{\begin{pmatrix} D_1\phi^{(1)} & D_1\phi^{(2)} \\ D_1\phi^{(3)} & D_1\phi^{(4)} \end{pmatrix}\cdot\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \begin{pmatrix} D_2\phi^{(1)} & D_2\phi^{(2)} \\ D_2\phi^{(3)} & D_2\phi^{(4)} \end{pmatrix}\cdot\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}\right\},$$

and treat $D_2\phi\cdot x$ by analogy. The $D_i\phi\cdot x$ are thus again two-row matrices. We now choose step sizes $h = \Delta r$, $k = \Delta t$ and provide the rectangle $Q = \{(r,t): 0 \leqq r \leqq R,\ 0 \leqq t \leqq T\}$ with the rectangular mesh

$$Q_\Delta = \{(i + \tfrac{1}{2})\cdot h,\ j\cdot k),\ i = 0 \ldots . N;\ j = 0, \ldots . M\}$$

with $(N + \frac{1}{2})\cdot h = R$, $M\cdot k = T$. All matrix, vector and scalar functions $\psi(r,t)$ are abbreviated:

$$\psi_{ij}: = \psi((i + \tfrac{1}{2})\cdot h,\ j\cdot k) = \psi(r_{i+1/2}, t_j)$$

The <u>linearized Crank-Nicholson method</u> now reads (see [2], [3])

$$\begin{aligned} G_i(W_{j+1}) \equiv &- \frac{\lambda}{2}\,\frac{2i}{2i+1}\,\bar{g}_{i-\frac{1}{2},j}\cdot(W_{i-1,j+1} - W_{i-1,j}) + \\ &+ \left[I + \frac{\lambda}{2}\cdot\left(\frac{2i}{2i+1}\,\overset{+}{g}_{i-\frac{1}{2},j} + \frac{2i+2}{2i+1}\,\bar{g}_{i+\frac{1}{2},j}\right)\right]\cdot(W_{i,j+1} - W_{ij}) \\ &- \frac{\lambda}{2}\,\frac{2i+2}{2i+1}\,\overset{+}{g}_{i+\frac{1}{2},j}\,(W_{i+1,j+1} - W_{i+1,j}) - \qquad (3) \\ &- \frac{2\lambda}{2i+1}\left[i\phi_{i-\frac{1}{2}j}W_{i-1,j} - (i\phi_{i-\frac{1}{2}j} + (i+1)\phi_{i+\frac{1}{2}j})W_{ij} + (i+1)\phi_{i+\frac{1}{2},j}W_{i+1,j}\right] = 0 \end{aligned}$$

for $i = 0, 1, \ldots, N-1$

where

$$\lambda = k \cdot h^{-2} , \quad W_{ij} = (U_{ij}, V_{ij})^T ,$$

$$W_j = (W_{o,j}, W_{1,j} \dots W_{N-1,j})^T \in \mathbb{R}^{2N} ,$$

$$\phi_{-\frac{1}{2},j} = 0 , \ \phi_{i-\frac{1}{2},j} = \phi \left(\tfrac{1}{2}(W_{i,j} + W_{i-1,j}), \tfrac{1}{h} (W_{i,j}-W_{i-1,j})\right) \ i=1,2,\dots N$$

$$g^-_{-\frac{1}{2},j} = g^+_{-\frac{1}{2},j} = 0$$

$$g^{\pm}_{i-\frac{1}{2},j} = \phi_{i-\frac{1}{2},j} \pm \tfrac{1}{2} D_1\phi_{i-\frac{1}{2},j} \cdot (W_{i,j} - W_{i-1,j}) + \tfrac{1}{h} D_2\phi_{i-\frac{1}{2},j} \cdot (W_{i,j}-W_{i-1,j})$$

$$i = 1,2\dots N$$

The quantities U_{ij}, V_{ij} are the numerically calculated approximations of the values of the exact solution $u_{i,j}$, $v_{i,j}$ at the mesh points $r_{i+\frac{1}{2}}, t_j$. For every time step one has to solve a system of linear equations of the form (3), where the unknown vector W_{j+1} has to be determined. The coefficient matrices of the system of equations (3) are block-tridiagonal with two-row blocks.

In [3] the following convergence theorem is proved:

<u>Theorem 1:</u> Let the initial boundary value problem (1*) - ($1\overset{*}{c}$) have in Q a uniquely determined, sufficiently smooth solution w(r,t) and let ϕ, W_A, W_R be sufficiently smooth. Furthermore, let the matrix

$$\Phi\ (x_1,x_2,y_1,y_2) := \phi\ (x_1,x_2,y_1,y_2) + D_2\phi(x_1,x_2,y_1,y_2)\cdot y$$

with $y = (y_1,y_2)^T$ satisfy the criterion:

$$\left.\begin{array}{l}\underline{\text{there is a fixed number } \gamma > 0 \text{ such that the symmetric matrices}}\\ \\ \qquad \underline{\Phi\ (x_1,x_2,y_1,y_2) + \Phi^T(x_1,x_2,y_1,y_2) - \gamma\cdot I}\\ \\ \underline{\text{are positive semi-definite for all } (x_1,x_2,y_1,y_2) \in \mathbb{R}^4\ .}\end{array}\right) \qquad (4)$$

Let the step sizes in the difference scheme (3) always be chosen such that for fixed constants $K_o > 0$, $K_1 > 0$ it holds that

$$K_o\ \Delta r \leq \frac{\Delta t}{\Delta r} \leq K_1 \qquad (5)$$

The solution of (3) then converges for $\Delta r,\Delta t \to 0$ at the grid points $(r_{i+\frac{1}{2}}, t_j)$ of Q_Δ to the exact solution of (1*), i.e. it holds that

$$\left.\begin{array}{l}\max\limits_{0\leq j\leq M} \left(\Delta r \cdot \sum\limits_{i=o}^{N} \left[(U_{ij}-u_{ij})^2 + (V_{ij}-v_{ij})^2\right]\right)^{1/2} \leq M\cdot(\Delta r)^2\\ \\ \qquad\qquad\qquad\qquad\qquad\qquad \text{for fixed } M > 0\end{array}\right) \qquad (6)$$

<u>Note:</u> The criterion (4) constitutes a generalization of the term "parabolic" to systems. If the differentiation on the RHS of eq. (1*) is performed, one obtains

$$\frac{\partial w}{\partial t} = \Phi \left(w, \frac{\partial w}{\partial r}\right) \cdot \frac{\partial^2 w}{\partial r^2} + \ldots .$$

This criterion thus states that the symmetric component of the coefficient matrix before the highest derivative with respect to space is uniformly positive definite; it also appears to be important in practice since the numerical calculations almost invariably break down, if it is not satisfied.

Another way of numerically solving (1*) is to use the <u>nonlinear Crank-Nicholson method:</u>

$$\frac{1}{\Delta t} (W_{i,j+1} - W_{ij}) = \frac{1}{2} \frac{1}{(i+1/2)\ \Delta r} \frac{1}{\Delta r} \cdot \Big[(i+1) \cdot \Delta r\ \phi_{i+\frac{1}{2},j} \frac{W_{i+1,j} - W_{ij}}{\Delta r} +$$

$$- i\ \Delta r \cdot \phi_{i-\frac{1}{2},j} \frac{W_{ij} - W_{i-1,j}}{\Delta r} + (i+1) \Delta r \phi_{i+\frac{1}{2},j+1} \frac{W_{i+1,j+1} - W_{i,j+1}}{\Delta r} +$$

$$- i\ \Delta r \phi_{i-\frac{1}{2},\ j+1} \frac{W_{ij+1} - W_{i-1,j+1}}{\Delta r} \Big],\ i = 0, \ldots .\ N - 1$$

or

$$F_i(W_{j+1}) \equiv - \frac{\lambda}{2} \frac{2i}{2i+2} \phi_{i-\frac{1}{2},j+1} W_{i-1,j+1} +$$

$$+ \Big[I + \frac{\lambda}{2} \Big(\frac{2i}{2i+1} \phi_{i-\frac{1}{2},j+1} + \frac{2i+2}{2i+1} \phi_{i+\frac{1}{2},j+1} \Big) \Big] W_{i,j+1} + \tag{7}$$

$$+ \Big[-I + \frac{\lambda}{2} \Big(\frac{2i}{2i+1} \phi_{i-\frac{1}{2},j} + \frac{2i+2}{2i+1} \phi_{i+\frac{1}{2},j} \Big) \Big] W_{i,j} +$$

$$- \frac{\lambda}{2} \frac{2i+2}{2i+1} \phi_{i+\frac{1}{2},j+1} W_{i+1,j+1} - \frac{\lambda}{2} \frac{2i}{2i+1} \phi_{i-\frac{1}{2},j} W_{i-1,j} - \frac{\lambda}{2} \frac{2i+2}{2i+1} \phi_{i+\frac{1}{2},j} W_{i+1,j} = 0$$

for i = 0, 1,... N-1

This scheme entails solving a system of nonlinear equations for every time step. One possibility is to use the multi-dimensional Newton method, which is treated in the next section.

3. THE NEWTON METHOD

A classical and reliable method of solving systems of equations is the Newton method, which is defined as follows:

Let $$F(x) = (F_1(x_1, \dots x_n), \dots\dots F_n(x_1, \dots x_n))^T$$

be a vector function whose partial derivatives exist and are continuous. It is required to find a solution $x^* = (x_1^*, \dots x_n^*)^T$ of the system of equations

$$F(x) = 0 \tag{8}$$

The method is then as follows:

1. Let $x^{(0)}$ be chosen as starting vector.
2. Let the systems of linear equations

$$\underline{F'(x^{(\nu)}) \cdot x^{(\nu+1)} = F'(x^{(\nu)}) \cdot x^{(\nu)} - F(x^{(\nu)})} \tag{9}$$

be solved for $x^{(\nu+1)}$ in the cases $\nu = 0.1, \dots \; k - 1$.

Here $F'(x^{(\nu)})$ is the functional matrix of $F(x)$ at the point $x^{(\nu)}$. In general, the Newton method is just locally convergent. If, however, $x^{(0)}$ is suitably chosen so that the system (9) converges, and if $F'(x^*)$ is a non-singular matrix and all second partial derivatives of $F(x)$ are also continuous in a vicinity of x^*, quadratic convergence occurs, i.e. it holds that

$$\| x^{(\nu+1)} - x^* \| \leq L \cdot \| x^{(\nu)} - x^* \|^2 , \quad \nu = 0,1,2,\ldots \tag{10}$$

where $L > 0$ is a constant and $\| \cdot \|$ is a vector norm. The expression (10) states that the convergence of the Newton method is extremely fast.

To apply the Newton iteration to the system of differential equations (7), first the functional matrix $F'(W)$ of the vector function

$F(W) = (F_o(W_o,\ldots W_{N-1}),\ldots F_{N-1}(W_o\ldots W_{N-1}))^T$ occurring in the system (7) has to be calculated. For the sake of simplicity, we omit the indices j,j+1 in the following and define

$$\frac{\partial F_i}{\partial W_k} := \begin{pmatrix} \dfrac{\partial F_i^{(1)}}{\partial U_k} & \dfrac{\partial F_i^{(1)}}{\partial V_k} \\ \dfrac{\partial F_i^{(2)}}{\partial U_k} & \dfrac{\partial F_i^{(2)}}{\partial V_k} \end{pmatrix} \quad \begin{array}{l} \text{for} \\ i,k = 0,1,\ldots, N-1 \end{array} \tag{11}$$

with $F_i = (F_i^{(1)}, F_i^{(2)})^T$, $W_k = (U_k,V_k)^T$.

As $F_i(W)$ in the system (7) only depends on the variables W_{i-1}, W_i, W_{i+1}, F(W) is a block-tridiagonal matrix in which the blocks are of the form (11). From the system (7) one now obtains by calculation (see notations in Sec. 2)

$$\frac{\partial F_i}{\partial W_{i-1}} = -\frac{\lambda}{2}\,\frac{2i}{2i+1}\cdot\begin{pmatrix} \dfrac{\partial\left[\phi^{(1)}_{i-1/2}(U_{i-1}-U_i)+\phi^{(2)}_{i-1/2}(V_{i-1}-V_i)\right]}{\partial U_{i-1}}, & \dfrac{\partial\left[\phi^{(1)}_{i-1/2}(U_{i-1}-U_i)+\phi^{(2)}_{i-1/2}(V_{i-1}-V_i)\right]}{\partial V_{i-1}} \\ \dfrac{\partial\left[\phi^{(3)}_{i-1/2}(U_{i-1}-U_i)+\phi^{(4)}_{i-1/2}(V_{i-1}-V_i)\right]}{\partial U_{i-1}}, & \dfrac{\partial\left[\phi^{(3)}_{i-1/2}(U_{i-1}-U_i)+\phi^{(4)}_{i-1/2}(V_{i-1}-V_i)\right]}{\partial V_{i-1}} \end{pmatrix}$$

$$= -\frac{\lambda}{2}\,\frac{2i}{2i+1}\cdot\left[\phi_{i-\frac{1}{2}} - \frac{1}{2}\,D_1\phi_{i-\frac{1}{2}}\cdot(W_i-W_{i-1}) + D_2\phi_{i-\frac{1}{2}}\,\frac{W_i - W_{i-1}}{h}\right] = -\frac{\lambda}{2}\,\frac{2i}{2i+1}\,g^{-}_{i-1/2}$$

and hence, restoring the index j,

$$\frac{\partial F_i(W_j)}{\partial W_{i-1,j}} = -\frac{\lambda}{2}\,\frac{2i}{2i+1}\,g^{-}_{i-\frac{1}{2}} \quad \text{for } i = 1,2\ldots N-1 \tag{12a}$$

Correspondingly, one has

$$\frac{\partial F_i(W_j)}{\partial W_{i+1,j}} = -\frac{\lambda}{2}\,\frac{2i+2}{2i+1}\,g^{+}_{i+\frac{1}{2},j} \quad \text{for } i = 0,1,\ldots N-2 \tag{12b}$$

For the diagonal blocks one obtains

$$\frac{\partial F_i(W_j)}{\partial W_{ij}} = I + \frac{\lambda}{2}\left(\frac{2i}{2i+1}\, g^{+}_{i-\frac{1}{2},j} + \frac{2i+2}{2i+1}\, g^{-}_{i+\frac{1}{2},j}\right) \text{ for } i = 0,\dots N-2$$

$$\frac{\partial F_{N-1}(W_j)}{\partial W_{N-1,j}} = I + \frac{\lambda}{2}\left(\frac{2N-2}{2N-1}\, g^{+}_{N-\frac{3}{2},j} + \frac{2N}{2N-1}\, \tilde{g}^{-}_{N-\frac{1}{2},j}\right) \tag{12c}$$

with $\tilde{g}^{-}_{N-\frac{1}{2},j} := \tilde{\phi}_{N-\frac{1}{2},j} - \frac{1}{2} D_1 \tilde{\phi}_{N-\frac{1}{2},j}\,(W_{N,j+1} - W_{N-1,j}) + D_2 \tilde{\phi}_{N-\frac{1}{2},j}\, \frac{W_{N,j+1} - W_{N-1,j}}{h}$

$$\tilde{\phi}_{N-\frac{1}{2},j} := \phi\left(\frac{1}{2}\,(W_{N,j+1} + W_{N-1,j}),\ \frac{1}{h}\,(W_{N,j+1} - W_{N-1,j})\right)$$

For the other derivatives one gets

$$\frac{\partial F_i(W_j)}{\partial W_{kj}} = 0 \quad \text{for} \quad |i-k| \geq 2 \tag{12d}$$

substituting the vector W_j for the vector W_{j+1} in eqs. (3) and (7) now yields the following relation:

$$G_i(W_j) - F_i(W_j) = \begin{cases} 0 & \text{for } i = 0,\dots N-2 \\ \frac{\lambda N}{2N-1}\, \delta_{N-1,j} & \text{for } i = N-1 \end{cases}$$

with

$$\delta_{N-1,j} := \tilde{\phi}_{N-\frac{1}{2},j} \cdot (W_{N,j+1} - W_{N-1,j}) - \phi_{N-\frac{1}{2},j}(W_{Nj} - W_{N-1,j}) - g^{+}_{N-\frac{1}{2},j}(W_{N,j+1} - W_{N,j}).$$

With convergence of the approximation solution it holds that

$$\delta_{N-1,j} = O(\Delta t)$$

Furthermore, the formulae (12) are used to obtain

$$G(W_{j+1}) - [F'(W_j) \cdot (W_{j+1}-W_j) + F\,(W_j)] = b_j$$

where the vector $b_j \in \mathbb{R}^{2N}$ is as follows:

$$b_j = (0,0,\ldots., 0, \frac{\lambda N}{2N-1} \cdot (\delta_{N-1,j} + [\bar{g}_{N-\frac{1}{2},j} - \tilde{g}_{N-\frac{1}{2}j}] \cdot [W_{N-1,j+1} - W_{N-1,j}]))^T$$

The system of equations (3) can thus be written in the form

$$G(W_{j+1}) \equiv F'(W_j) \cdot [W_{j+1}-W_j] + F\,(W_j) + b_j = 0 \qquad (3^*)$$

Comparison with the system (9) shows that the scheme (3) - apart from the last block component - constitutes a Newton iteration for the system of nonlinear equations (7).

It has thus been shown that

Theorem 2: The linearized Crank-Nicholson scheme (3) is essentially identical with a Newton iteration for approximate solution of the Crank-Nicholson discretization (7), the approximate solution W_j at the old time t_j being taken as starting vector.

Note: In the linear case ϕ = const it immediately follows that $b_j = 0$, which it has to be.

When applied to the system (7), the Newton method (9) is

1. Let $(W_o^{(o)}, \dots W_{N-1}^{(o)})^T := (W_{oj} \dots W_{N-1,j})^T$ be chosen as starting vector.
2. Let the following system of equations be solved for the values

   $\nu = 0,1 \dots K-1$:

$$B_o^{(\nu)} \cdot W_o^{(\nu+1)} - C_o^{(\nu)} \cdot W_1^{(\nu+1)} = B_o^{(\nu)} \cdot W_o^{(\nu)} - C_o^{(\nu)} W_1^{(\nu)} - W_o^{(\nu)} + W_o^{(o)} + D_o^{(\nu)},$$

$$- A_i^{(\nu)} W_{i-1}^{(\nu+1)} + B_i^{(\nu)} W_i^{(\nu+1)} - C_i^{(\nu)} W_{i+1}^{(\nu+1)} =$$

$$= - A_i^{(\nu)} W_{i-1}^{(\nu)} + B_i^{(\nu)} W_i^{(\nu)} - C_i^{(\nu)} W_{i+1}^{(\nu)} - W_i^{(\nu)} + W_i^{(o)} + D_i^{(\nu)} \tag{13}$$

for $i = 1,2, \dots N-2$

$$- A_{N-1}^{(\nu)} W_{N-2} + \tilde{B}_{N-1,N-1}^{(\nu)} = - A_{N-1}^{(\nu)} W_{N-2}^{(\nu)} + \tilde{B}_{N-1}^{(\nu)} W_{N-1}^{(\nu)} - W_{N-1}^{(\nu)} + W_{N-1}^{(o)}$$

$$+ \tilde{D}_{N-1}^{(\nu)}$$

3. Let $(W_{oj+1}, \dots W_{N-1,j+1})^T := (W_o^{(k)}, \dots W_{N-1}^{(k)})^T$

Here the coefficient matrices in the scheme (13) are defined as follows:

$$A_i^{(\nu)} := \frac{\lambda i}{2i+1} \, g_{i-1/2}^{-(\nu)} \quad \text{for } i = 1, \dots N-1 \, ,$$

$$B_i^{(\nu)} := I + \frac{\lambda}{2i+1} \left(i \, g_{i-1/2}^{+(\nu)} + (i+1) g_{i+1/2}^{-(\nu)} \right) \quad \text{for } i = 1, \dots N-2,$$

$$\tilde{B}_i^{(\nu)} := I + \frac{\lambda}{2N-1} \left((N-1) g_{N-3/2}^{+(\nu)} + N \tilde{g}_{N-1/2}^{-(\nu)} \right),$$

$$C_i^{(\nu)} := \frac{\lambda(i+1)}{2i+1} \cdot g_{i+1/2}^{+(\nu)} \quad \text{for } i = 0, \dots N-2$$

$$D_i^{(\nu)} := \frac{\lambda}{2i+1} \Big[(i+1)\phi^{(\nu)}_{i+1/2} \left(W^{(\nu)}_{i+1} - W^{(\nu)}_{i}\right) - i\phi^{(\nu)}_{i-1/2} \left(W^{(\nu)}_{i} - W^{(\nu)}_{i-1}\right) +$$

$$+ (i+1)\phi^{(o)}_{i+1/2} \left(W^{(o)}_{i+1} - W^{(o)}_{i}\right) - i\phi^{(o)}_{i-1/2} \left(W^{(o)}_{i} - W^{(o)}_{i-1}\right)\Big] \quad \text{for } i=0,\ldots N-2$$

$$\tilde{D}^{(\nu)}_{N-1} := \frac{\lambda}{2N-1} \Big[N\tilde{\phi}^{(\nu)}_{N-1/2} \left(W^{(\nu)}_{Nj+1} - W^{(\nu)}_{N-1}\right) - (N-1)\phi^{(\nu)}_{N-3/2} \left(W^{(\nu)}_{N-1} - W^{(\nu)}_{N-2}\right) +$$

$$+ N\phi^{(o)}_{N-1/2} \left(W^{(o)}_{Nj} - W^{(o)}_{N-1}\right) - (N-1)\phi^{(o)}_{N-3/2} \left(W^{(o)}_{N-1} - W^{(o)}_{N-2}\right)\Big].$$

Here the $g^{\pm(\nu)}_{i\pm 1/2}$, $\phi^{(\nu)}_{i\pm 1/2}$ define the function values obtained by inserting the arguments $W^{(\nu)}_i$, $i = 0,1,\ldots N-1$. It should be recalled that the symbols $\tilde{g}_{N-1/2}$, $\tilde{\phi}_{N-1/2}$ were defined just after formula (12c).

Finally, the convergence order of the Newton scheme (13) should be considered heuristically: The functional matrix of the system of equations (7) is of the following form (the indices j being omitted for simplicity) owing to (12):

$$F'(W) = I + \frac{\lambda}{2} H(W)$$

where the 2N-row matrix $H = H(W)$ is

$$H = \begin{pmatrix}
2g^-_{1/2} & -2g^+_{1/2} & & & \\
-\frac{2}{3}g^-_{1/2} & \frac{2}{3}g^+_{1/2} + \frac{4}{3}g^-_{3/2} & -\frac{4}{3}g^+_{3/2} & & O \\
\ddots & \ddots & \ddots & & \\
& -\frac{2i}{2i+1}g^-_{i-1/2} & \frac{2i}{2i+1}g^+_{i-1/2} + \frac{2i+2}{2i+1}g^-_{i+1/2} & -\frac{2i+2}{2i+1}g^+_{i+1/2} & \\
& \ddots & \ddots & \ddots & \\
O & & & & -\frac{2N-2}{2N-3}g^+_{N-\frac{3}{2}} \\
& & & -\frac{2N-2}{2N-1}g^-_{N-\frac{3}{2}} & \frac{2N-2}{2N-1}g^+_{N-\frac{3}{2}} + \frac{2N}{2N+1}\tilde{g}^-_{N-1/2}
\end{pmatrix}$$

In [3], Sec. 4 (see lemma 2, formula (13a)), the following estimate is proved:

$$\| \hat{D} \cdot (I + \frac{\lambda}{2} H(w_{j+1}))^{-1} \cdot \hat{D}^{-1} \| \leq 1 + \tilde{k}\, \Delta t \qquad (15)$$

Here $\tilde{k} > 0$ is fixed, $\hat{D}$ is a certain diagonal matrix, the norm occurring is the spectral norm, and w_{j+1} is the vector of the exact solution values at time t_{j+1}. From (15) it follows in particular that F is non-singular.

On the basis of the numerical experiments [4] it can be assumed that the approximation solution W_{j+1} obtained by means of the scheme (13) converges for Δr, $\Delta t \to 0$ to the exact solution $w\,(r, t_{j+1})$ of (1) at the mesh points (the exact mathematical proof of convergence is not yet available). For reasons of continuity it can then be concluded by means of (15) that $F'(W_{j+1})$ is also non-singular for sufficiently small step sizes Δr, Δt, which, however, means quadratic convergence of the Newton scheme (13).

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