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APPROXIMATION AND NUMERICAL RESULTS FOR PHASE FIELD SYSTEM BY A FRACTIONAL STEP SCHEME

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1. INTRODUCTION

We consider the phase field system

(1.1) $$\tau\varphi_t = \xi^2\Delta\varphi + \frac{1}{2a}\left(\varphi - \varphi^3\right) + 2u, \quad \text{in} \quad Q_T = (0,T)\times\Omega,$$

(1.2) $$\left(u+\frac{l}{2}\varphi\right)_t = k\Delta u, \quad \text{in} \quad Q_T,$$

subject to the Dirichlet boundary conditions and initial conditions

(1.3) $$\varphi|_\Sigma = u|_\Sigma = 0, \quad \text{in} \quad \Sigma = (0,T)\times\partial\Omega,$$

(1.4) $$\varphi(0,x) = \varphi_0(x), \quad u(0,x) = u_0(x), \quad \text{on} \quad \partial\Omega,$$

where Ω is a bounded domain in $\mathbf{R}^n$ with smooth boundary $\partial\Omega$, and φ, u, τ, ξ, l and k are as in [9], [11].

Setting

(1.5) $$y = u + \frac{l}{2}\varphi,$$

system (1.1)–(1.4) takes the form

(1.6) $$y_t - k\Delta y + \frac{kl}{2}\Delta\varphi = 0,$$

(1.7) $$\varphi_t - \frac{\xi^2}{\tau}\Delta\varphi + \frac{1}{\tau}\left(l - \frac{1}{2a}\right)\varphi + \frac{1}{2a\tau}\varphi^3 - \frac{2}{\tau}y = 0,$$

(1.8) $$y|_\Sigma = \varphi|_\Sigma = 0,$$

(1.9) $$y(0,x)=y_0(x)=u_0(x)+\frac{l}{2}\varphi_0(x),\ \varphi(0,x)=\varphi_0(x).$$

Let $X=L^2(\Omega)\times L^2(\Omega)$. Then X is a real Banach space with respect to the norm $\|\cdot\|$ defined by

$$\left\|\begin{pmatrix} y\\ \varphi\end{pmatrix}\right\|=\|y\|_{L^2(\Omega)}+\|\varphi\|_{L^2(\Omega)}.$$

Define the operator $A: D(A)\subset X\to X$ by

$$A\begin{pmatrix} y\\ \varphi\end{pmatrix}=\begin{pmatrix} -k\Delta y+k\frac{l}{2}\Delta\varphi\\ -\frac{\xi^2}{\tau}\Delta\varphi+\frac{1}{\tau}\left(l-\frac{1}{2a}\right)\varphi\end{pmatrix},$$

$$D(A)=\begin{pmatrix} H_0^1(\Omega)\cap H^2(\Omega)\\ H_0^1(\Omega)\cap H^2(\Omega)\end{pmatrix},$$

and the operator $B: D(B)\subset X\to X$:

$$B\begin{pmatrix} y\\ \varphi\end{pmatrix}=\begin{pmatrix} 0\\ (2a\tau)^{-1}\varphi^3-\frac{2}{\tau}y\end{pmatrix},$$

$$D(B)=\left\{\begin{pmatrix} y\\ \varphi\end{pmatrix}\in X; (2a\tau)^{-1}\varphi^3-\frac{2}{\tau}y\in L^6(\Omega)\right\}$$

Thus, system (1.6)–(1.7) can be rewritten in the form

(S) $$\frac{\partial}{\partial t}\begin{pmatrix} y\\ \varphi\end{pmatrix}+A\begin{pmatrix} y\\ \varphi\end{pmatrix}+B\begin{pmatrix} y\\ \varphi\end{pmatrix}=0.$$

For others settings into the abstract framework of the phase-field equations (1.1)–(1.4) see, e.g., [6], [14].

The idea behind the Lie-Trotter scheme (known as the method of fractional step in numerical approximation of PDE's) is to decompose the original problem into several simpler problems.

Here we associate to system (S) the following approximating scheme

(1.10) $$\begin{pmatrix} y_\varepsilon(t)\\ \varphi_\varepsilon(t)\end{pmatrix}'+A\begin{pmatrix} y_\varepsilon(t)\\ \varphi_\varepsilon(t)\end{pmatrix}=0,\ \ in\ [i\varepsilon,(i+1)\varepsilon],$$

(1.11) $$\varphi_\varepsilon(i\varepsilon)=z_\varepsilon((i+1)\varepsilon),\ i=0,1,\dots,M-1,$$

(1.12) $$z'_\varepsilon(t)+B\begin{pmatrix} y_\varepsilon(t)\\ z_\varepsilon(t)\end{pmatrix}=0,\ \ \text{in } [i\varepsilon,(i+1)\varepsilon],$$

(1.13) $$z_\varepsilon(i\varepsilon)=\varphi_\varepsilon^+(i\varepsilon),\ i=0,1,\dots,M-1,$$

where $0<\varepsilon<\dots<M\varepsilon=T$ is a partition of the time-interval $[0,T]$, $\varphi_\varepsilon^+(i\varepsilon)$ is the right limit of φ_ε at $i\varepsilon$. We assume the following convention: $\varphi_\varepsilon^+(0)=\varphi_0$, $y_\varepsilon(0)=y_0$.

Recall that $J: X\to X^*$ is the *duality mapping* of the space X (see, for instance, [2]) and that $A\subset X\times X$ is:

accretive, if for every pair $[x_1,y_1],[x_2,y_2]\in A$, there exist $w\in J(x_1-x_2)$ such that

(*i*) $$<y_1-y_2,w>\ \geq 0,$$

or, equivalently,

(*ii*) $$\|x_1-x_2\|\leq\|x_1-x_2+\lambda(y_1-y_2)\|,\ (\forall)\lambda>0,\ [x_i,y_i]\in A,\ i=1,2,$$

m-accretive, if it is accretive and $R(I+A)=X$,
ω*-accretive*, if $A+\omega I$ is accretive, where $\omega\in\mathbb{R}$,
ω*-m-accretive*, if $A+\omega I$ is m-accretive,

where $<\cdot,\cdot>$ is the pairing between X and X^* (the dual space of X), I is the identity operator in X, $R(A)$ is the range of A.

Another convenient way to define the accretiveness is obtained using $[\cdot,\cdot]_S$ - the directional derivative of the norm

$$[x,y]_S=\lim_{\lambda\downarrow 0}\frac{\|x+\lambda y\|-\|x\|}{\lambda},\qquad x,y\in X,$$

i.e., (ii) can be equivalently written as

(*ii'*) $$[x_1-x_2,y_1-y_2]_S\geq 0,\ \ (\forall)\ [x_i,y_i]\in A,\ i=1,2.$$

(see also [2], [15], [16]). Recall that if X is a real Hilbert space then $[x,y]_S=\ <x,y>$ $\forall x,y\in X$ (see [16], Remark 1.4.1).

It is well known that, under certain hypotheses on A, the Cauchy problem

$$\begin{cases} v'(t)+Av(t)\ni 0, t\geq 0\\ v(0)=v_0\end{cases}$$

has a generalized solution $v \in C([0,\infty),X)$ given by the exponential formula

$$v(t)=\lim_{t\to\infty}\left(I+\frac{t}{n}A\right)^{-n},\ (\forall)t\geq 0,$$

for every $v_0 \in \overline{D(A)}$ (a classical result of Crandall-Ligget, see, e.g., [2]).

This is the sense in which we will treat the problems (1.6)–(1.9) and (1.10)–(1.13).

2. CONVERGENCE OF THE APPROXIMATE SCHEME

Let us recall the following result due to Barbu and Iannelli ([5]).

THEOREM 2.1. *Let Y be a real Banach space, let C be a closed subset of Y and $K = C \cap D(A)$ be a convex subset of Y such that*

(H1) *A is ω-accretive and* $R(I+\lambda A)\supset \overline{D(A)}$, $(\forall)\lambda\in(0,\lambda_0)$;

(H2) *B is a continuous ω-accretive operator on C such that*

$$R(I+\lambda B)\supset C,\ (\forall)\lambda\in(0,\lambda_0);$$

(H3) $R(I+\lambda(A+B))\supset K$, $(I+\lambda A)^{-1}K\subset K$, $(I+\lambda B)^{-1}K\subset K$;

(H4) *For every* $[x,y]\in A$, *there exists* $\{x_h\}\subset Y$ *such that*

$$\lim_{h\to 0}x_h=x,\qquad \lim_{h\to 0}\left\|\frac{1}{h}\left(x_h-e^{-Ah}x_h\right)-y\right\|=0$$

Then, for every $y_0\in K$, *we have*

$$\lim_{\varepsilon\to 0}y_\varepsilon(t)=y(t),\ (\forall)t\geq 0,$$

and the limit is uniform on bounded t intervals.

Here, by $y(t)$, we have denoted the generalized solution to the Cauchy problem:

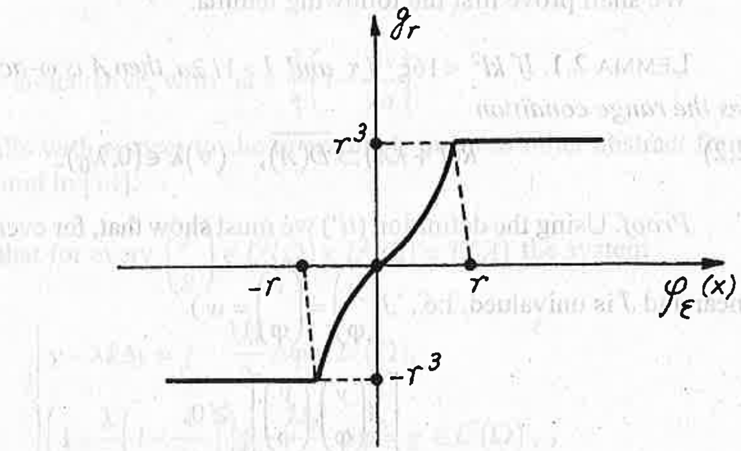
$$\begin{cases} y'(t)+Ay(t)+By(t)\ni 0, & t\in(0,T)\\ y(0)=y_0\end{cases}$$

and by $y_\varepsilon(t)$ the solution of the corresponding approximative scheme.

This result is not applicable to the problem (1.10)–(1.13) because we cannot find a subset C as in (H2) and such that the operator B be continuous on C.

Therefore, we will replace the operator B with another one having all the properties required by Theorem 2.1 and we will show that the approximate solution $\begin{pmatrix} y_\varepsilon\\ \varphi_\varepsilon\end{pmatrix}$ corresponding to this new operator is in fact an approximate solution corresponding to B (see Remark 3.1, below). Namely, we consider the operator B_r defined by (see also Figure 1)

Fig. 1



$$B_r: L^2(\Omega)\times L^2(\Omega)\to L^2(\Omega)\times L^\infty(\Omega)\subset L^2(\Omega)\times L^2(\Omega),$$

$$B_r\begin{pmatrix} y_\varepsilon\\ \varphi_\varepsilon\end{pmatrix}=\begin{pmatrix} 0\\ (2a\tau)^{-1}g_r(\varphi_\varepsilon(x))-\dfrac{2}{\tau}y_\varepsilon(x)\end{pmatrix},$$

where

$$g_r(\varphi_\varepsilon)=\begin{cases}\varphi_\varepsilon^3(x), & |\varphi_\varepsilon(x)|<r,\\ +r^3, & \varphi_\varepsilon>+r,\\ -r^3, & \varphi_\varepsilon<-r,\end{cases}$$

Substituting in (S) and in (2.12) $B\begin{pmatrix} y_\varepsilon(t)\\ \varphi_\varepsilon(t)\end{pmatrix}$ by $B_r\begin{pmatrix} y_\varepsilon(t)\\ \varphi_\varepsilon(t)\end{pmatrix}$ we obtain:

$$(S')\qquad \frac{\partial}{\partial t}\begin{pmatrix} y\\ \varphi\end{pmatrix}+A\begin{pmatrix} y\\ \varphi\end{pmatrix}+B_r\begin{pmatrix} y\\ \varphi\end{pmatrix}=0,$$

$$(2.1)\qquad z'_\varepsilon(t)+B_r\begin{pmatrix} y_\varepsilon(t)\\ \varphi_\varepsilon(t)\end{pmatrix}=0,\ \text{in}\ \ [i\varepsilon,(i+1)\varepsilon].$$

We associate to system (S') the approximating scheme (1.10), (1.11), (2.1) and (1.13).

Now we prove

PROPOSITION 2.1. *If* $kl^2 < 16\xi^2/\tau$ *and* $l > 1/2a$ *then, the operators* A, B_r *and* $Y = C = K = L^2(\Omega)\times L^2(\Omega)$ *satisfy all the hypotheses of Theorem 2.1.*

We shall prove first the following lemma.

LEMMA 2.1. *If* $kl^2 < 16\xi^2/\tau$ *and* $l > 1/2a$ *then* A *is* ω*-accretive and satisfies the range condition*

(2.2) $$R(I+\lambda A)\supset \overline{D(A)},\quad (\forall)\lambda\in(0,\lambda_0).$$

Proof. Using the definition (ii') we must show that, for every $\begin{pmatrix} y\\ \varphi\end{pmatrix}\in X$, ($A$ is linear and J is univalued, i.e., $J\begin{pmatrix} y\\ \varphi\end{pmatrix}=\begin{pmatrix} y\\ \varphi\end{pmatrix}=w$)

$$\left[A\begin{pmatrix} y\\ \varphi\end{pmatrix},\begin{pmatrix} y\\ \varphi\end{pmatrix}\right]_S\geq 0.$$

Using Green formula and Cauchy-Schwarz's inequality, we get (X is real Hilbert space)

$$\left\langle\begin{pmatrix} -k\Delta y+\dfrac{kl}{2}\Delta\varphi\\ -\dfrac{\xi^2}{\tau}\Delta\varphi+\dfrac{1}{\tau}\left(l-\dfrac{1}{2a}\right)\varphi\end{pmatrix},\begin{pmatrix} y\\ \varphi\end{pmatrix}\right\rangle=$$

$$=k\|\nabla y\|^2_{L^2(\Omega)}-\frac{kl}{2}\langle\nabla y,\nabla\varphi\rangle_{L^2(\Omega)}+\frac{\xi^2}{\tau}\|\nabla\varphi\|^2_{L^2(\Omega)}+\frac{1}{\tau}\left(l-\frac{1}{2a}\right)\|\varphi\|^2_{L^2(\Omega)}\geq$$

$$\geq k\|\nabla y\|^2_{L^2(\Omega)}-\frac{kl}{2}\|\nabla y\|_{L^2(\Omega)}\cdot\|\nabla\varphi\|^2_{L^2(\Omega)}+\frac{\xi^2}{\tau}\|\nabla\varphi\|^2_{L^2(\Omega)}+\frac{1}{\tau}\left(l-\frac{1}{2a}\right)\|\varphi\|^2_{L^2(\Omega)}.$$

Since $kl^2<16\xi^2/\tau$ then $k^2l^2/4-4k\xi^2/\tau\leq 0$ and then

$$k\|\nabla y\|^2_{L^2(\Omega)}-\frac{kl}{2}\|\nabla y\|_{L^2(\Omega)}\cdot\|\nabla\varphi\|^2_{L^2(\Omega)}+\frac{\xi^2}{\tau}\|\nabla\varphi\|^2_{L^2(\Omega)}\geq 0.$$

Thus, because $l>1/2a$,

$$\left\langle A\begin{pmatrix} y\\ \varphi\end{pmatrix},w\right\rangle\geq\frac{1}{\tau}\left(l-\frac{1}{2a}\right)\|\varphi\|^2_{L^2(\Omega)}\geq-\frac{1}{\tau}\left(l-\frac{1}{2a}\right)\left(\|y\|_{L^2(\Omega)}+\|\varphi\|_{L^2(\Omega)}\right)^2,$$

i.e.

$$\left\langle A\begin{pmatrix} y\\ \varphi\end{pmatrix}+\frac{1}{\tau}\left(l-\frac{1}{2a}\right)\begin{pmatrix} y\\ \varphi\end{pmatrix},w\right\rangle\geq 0$$

Hence A is ω-accretive, with $\omega=\dfrac{1}{\tau}\left(l-\dfrac{1}{2a}\right)$.

Other results with respect to the operator A, put into other abstract framework, can be found in [14].

It is clear that for every $\begin{pmatrix} f\\ g\end{pmatrix}\in L^2(\Omega)\times L^2(\Omega)=\overline{D(A)}$ the system

$$\begin{cases} y-\lambda k\Delta y=j-\dfrac{\lambda kl}{2}\Delta\varphi\in L^2(\Omega),\\ \left(1+\dfrac{\lambda}{\tau}\left(l-\dfrac{1}{2a}\right)\right)\varphi-\dfrac{\lambda\xi^2}{\tau}\Delta\varphi=g\in L^2(\Omega),\end{cases}$$

has a unique solution $\begin{pmatrix} y\\ \varphi\end{pmatrix}\in D(A)$ for λ small (see [1], [4], [7]; Ω is supposed to be, as in Theorem 4.1, pp. 131, [4]). Thus (2.2) is true.

The proof of Proposition 2.1. By Proposition 3.9 pp. 110 ([2]), we have that $A+B_r$ is m-accretive and surjective. Taking into account Lemma 2.1 and because A is single valued and the semigroup e^{-At} is differentiable on $D(A)$ (see [3]), we remark that all the hypotheses of Theorem 2.1 are fulfilled and therefore the proof of Proposition 2.1 is complete.

Remark 2.1. If we can choose r such that $\|\varphi_\varepsilon(x)\|_{L^\infty(\Omega)}\leq r$, a.e. $x\in\Omega$ then

$$B\begin{pmatrix} y_\varepsilon(t)\\ \varphi_\varepsilon(t)\end{pmatrix}=B_r\begin{pmatrix} y_\varepsilon(t)\\ \varphi_\varepsilon(t)\end{pmatrix}$$

and the solution of the approximate problem (S')+(2.1) is in fact the solution of the approximate problem $(S)'+(1.12)$.

3. NUMERICAL RESULTS

We consider $n=1$ and $\Omega=[0,c]\subset \mathbf{R}_+$. For the space interval we use the grid with equidistant nodes

$$0<x_0<x_1<\ldots<x_{N-1}<x_N=c.$$

Denote by $\begin{pmatrix} y_{i,j} \\ fi_{i,j} \end{pmatrix}$ the approximated matrix for $\begin{pmatrix} y \\ \varphi \end{pmatrix}$, where

$$y_{i,j}=y(t_i,x_j),\quad i=\overline{1,M},\quad j=\overline{1,N},$$

$$fi_{i,j}=\varphi(t_i,x_j),\quad i=\overline{1,M},\quad j=\overline{1,N}.$$

As well, we denote by $\begin{pmatrix} y\varepsilon_{i,j} \\ fi\varepsilon_{i,j} \end{pmatrix}$ the approximative matrix for $\begin{pmatrix} y_\varepsilon \\ \varphi_\varepsilon \end{pmatrix}$ where

$$y\varepsilon_{i,j} = y_\varepsilon(t_i,x_j),\quad i=\overline{1,M},\quad j=\overline{1,N},$$

$$\varphi\varepsilon_{i,j} = \varphi_\varepsilon(t_i,x_j),\quad i=\overline{1,M},\quad j=\overline{1,N}.$$

Using a standard implicit scheme, (1.6)–(1.7) are discretized as

(3.1)
$$\frac{\varphi_{i+1,j}-\varphi_{i,j}}{\varepsilon}-\frac{\xi^2}{\tau}\frac{\varphi_{i+1,j+1}-2\varphi_{i+1,j}+\varphi_{i+1,j-1}}{h^2}+$$
$$+\frac{1}{\tau}\left(l-\frac{1}{2a\tau}\right)\varphi_{i+1,j}+\frac{1}{2a}\varphi^3_{i+1,j}-\frac{2}{\tau}y_{i+1,j}=0,\quad i=\overline{0,M-1},\quad j=\overline{1,N-1},$$

(3.2)
$$\frac{y_{i+1,j}-y_{i,j}}{\varepsilon}-k\cdot\frac{y_{i+1,j+1}-2y_{i+1,j}+y_{i+1,j-1}}{h^2}+$$
$$+\frac{kl}{2}\frac{\varphi_{i+1,j+1}-2\varphi_{i+1,j}+\varphi_{i+1,j-1}}{h^2}=0,\quad i=\overline{0,M-1},\quad j=\overline{1,N-1},$$

and

$$\varphi_{i,0}=\varphi_{i,N}=0,\quad y_{i,0}=y_{i,N}=0,\quad i=\overline{1,M},$$

$$\varphi_{0,j}=\varphi_0(x_j),\quad y_{0,j}=y_0(x_j)=0,\quad j=\overline{1,N},$$

where $h=x_{i+1}-x_i$

Setting

$$c_1=\xi^2/\tau h^2,\ c_2=\varepsilon/2a\tau-l\varepsilon/2-2\varepsilon\cdot c_1-1,\ c_3=\varepsilon\cdot c_1,$$
$$c_4=2\varepsilon/\tau,\ c_5=k\varepsilon/h^2,\ c_6=-2\cdot c_5-1,$$
$$c_7=-kl\varepsilon/2h^2,\ c_8=-c_7/2,\ c_9=-c_4/4a,$$

(3.1) and (3.2) can be rewritten for the level of time i, $i=\overline{1,M-1}$, in matrix form

(3.3)
$$\begin{pmatrix} \overline{A}_{11} & \overline{A}_{12} \\ \overline{A}_{21} & \overline{A}_{22} \end{pmatrix}\begin{pmatrix} \varphi_{i,j} \\ y_{i,j} \end{pmatrix}+\begin{pmatrix} \mathrm{diag}\ (c_9\cdot\varphi^3_{i,j}) & 0 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} \varphi_{i,j} \\ y_{i,j} \end{pmatrix}=d\ .$$

with $\overline{A}_{11},\overline{A}_{12},\overline{A}_{21},\overline{A}_{22}$, of $(N-1)\times(N-1)$ dimension, given by

$$\overline{A}_{11}=\begin{pmatrix} c_2 & c_1 & . & . & 0 \\ c_3 & c_2 & c_1 & . & 0 \\ . & . & . & . & c_1 \\ 0 & . & . & c_3 & c_2 \end{pmatrix}\qquad \overline{A}_{12}=\begin{pmatrix} c_4 & 0 & . & 0 \\ 0 & c_4 & . & 0 \\ . & . & . & . \\ 0 & . & . & c_4 \end{pmatrix}$$

$$\overline{A}_{21}=\begin{pmatrix} c_8 & c_7 & . & 0 \\ c_7 & . & . & . \\ . & . & . & c_7 \\ 0 & . & c_7 & c_8 \end{pmatrix}\qquad \overline{A}_{22}=\begin{pmatrix} c_6 & c_5 & . & 0 \\ c_5 & . & . & . \\ . & . & . & c_5 \\ 0 & . & c_5 & c_6 \end{pmatrix},$$

and $d=(d_1;d_2)=(-\varphi_{i,1},-\varphi_{i,2},\ldots,-\varphi_{i,N-1};-y_{i,1},-y_{i,2},\ldots,-y_{i,N-1})$.

Let $w=(f_i,y)$ denote the vector-solution for level of time i, i.e.

$$w=(\varphi_{i,1},\varphi_{i,2},\ldots,\varphi_{i,N-1};y_{i,1},y_{i,2},\ldots,y_{i,N-1}).$$

System (3.3) takes the form

(3.4)
$$\begin{cases} \overline{A}_{11}\varphi+\overline{A}_{12}y+g(\varphi)=d_1 \\ \overline{A}_{21}\varphi+\overline{A}_{22}y=d_2 \end{cases}$$

where $g(\varphi)=\mathrm{diag}(c_9\cdot\varphi^3_{i,j})_{i=\overline{1,N-1}}$.

Thus we have to solve the nonlinear system

$$F(w) = 0.$$

Using the Newton iterative method to solve it, we have

(3.5) $$w^{(j+1)} = w^{(j)} - F\left(w^{(j)}\right) / F'\left(w^{(j)}\right),$$

where

$$F(w) = \begin{pmatrix} \overline{A}_{11}\varphi + \overline{A}_{12}y + g(\varphi i) - d_1 \\ \overline{A}_{21}\varphi + \overline{A}_{22}y - d_2 \end{pmatrix},$$

$$F'(w) = \begin{pmatrix} \overline{A}_{11} + \operatorname{diag}\left(3 \cdot c_9 \cdot \varphi_{i,j}^2\right)_{i=\overline{1,N-1}} & \overline{A}_{12} \\ \overline{A}_{21} & \overline{A}_{22} \end{pmatrix}.$$

Using an implicit scheme and the Newton iterative method, we obtain from (2.1)

(3.6) $$\begin{cases} z_\varepsilon^{(j+1)}((i+1)\varepsilon) = z_\varepsilon^{(j)}((i+1)\varepsilon) - G\left(z_\varepsilon^{(j)}((i+1)\varepsilon)\right) / G'\left(z_\varepsilon^{(j)}((i+1)\varepsilon)\right), \\ z_\varepsilon^{0}((i+1)\varepsilon) = \varphi_\varepsilon^{+}(i\varepsilon), \end{cases}$$

where

$$G(z) = \frac{\varepsilon}{2a\tau} g_r(z) + z - \varphi_\varepsilon^{+}(i\varepsilon) - \frac{2}{\tau} y_\varepsilon(i\varepsilon).$$

Using the very same way of discretization and implicit scheme, the approximative version of (1.10) is given by

(3.7) $$\begin{pmatrix} \overline{A}_{11} & 0 \\ \overline{A}_{21} & \overline{A}_{22} \end{pmatrix} \begin{pmatrix} \varphi\varepsilon_{i,j} \\ y\varepsilon_{i,j} \end{pmatrix} = d\varepsilon$$

and

$$\varphi\varepsilon_{i,0} = \varphi\varepsilon_{i,N} = 0,\ y\varepsilon_{i,0} = y\varepsilon_{i,N} = 0,\ i = \overline{1,M},$$

$$\varphi\varepsilon_{0,j} = z_\varepsilon(0) = \varphi_\varepsilon^{+}(0) = \varphi_0(x_j),\ y\varepsilon_{0,j} = u_0(x_j) + \frac{l}{2}\varphi\varepsilon_{0,j},\ j = \overline{0,N},$$

with $d\varepsilon = \left(-\varphi\varepsilon_{i,1}, -\varphi\varepsilon_{i,2}, \ldots, -\varphi\varepsilon_{i,N-1}, -y\varepsilon_{i,1}, -y\varepsilon_{i,2}, \ldots, -y\varepsilon_{i,N-1}\right)$.

For fixed i $(i \geq 0)$, the computation of the approximate solution by fractional step method can be illustrated as in Figure 2

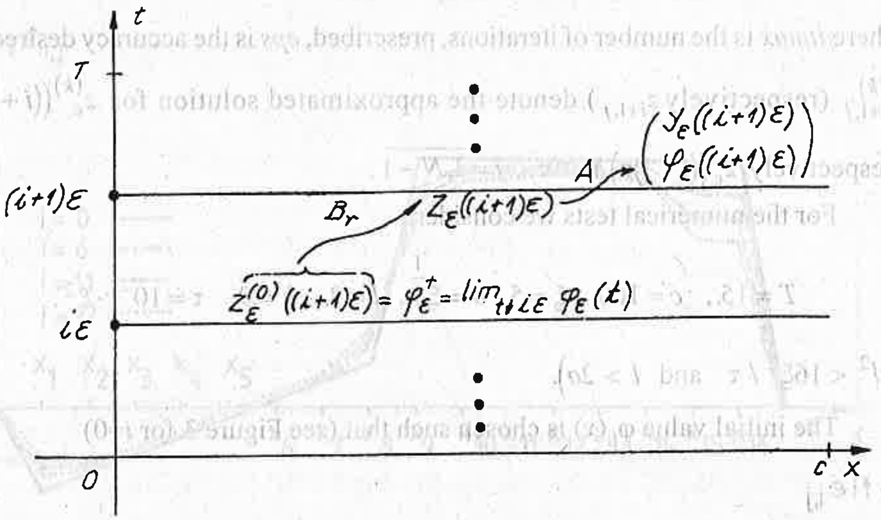


Fig. 2

and, the numerical algorithm to calculate it, can be obtained by the following sequence

$$z_{i+1,j}^{(0)} = \varphi\varepsilon_{i,j},\ j = \overline{1,N-1},$$

$$\downarrow$$

for $k = 1$ step 1 by 1 until itmax do

$$z_{i+1,j}^{(k+1)} = z_{i+1,j}^{(k)} - G\left(z_{i+1,j}^{(k)}\right) / G'\left(z_{i+1,j}^{(k)}\right),\ j = \overline{1,N-1},$$

$$\downarrow$$

if $\left[\sum_{j=1}^{N-1}\left(z_{i+1,j}^{(k+1)} - z_{i+1,j}^{(k)}\right)^2\right]^{\frac{1}{2}} \leq \text{eps}$ and $k < \text{itmax} \xrightarrow{\text{(false)}}$ STOP

$\downarrow$ (true)

$$z_{i+1,j} = z_{i+1,j}^{(k+1)},\ j = \overline{1,N-1},\ \text{goto sol},$$

next k

sol: $\downarrow$

$$\varphi\varepsilon_{i,j} = z_{i+1,j},\ j = \overline{1,N-1},$$

$$\downarrow$$

Solve the linear system (3.7)

$$\downarrow$$

$$\begin{pmatrix} y\varepsilon_{i+1,j} \\ \varphi\varepsilon_{i+1,j} \end{pmatrix},\ j = \overline{1,N-1},$$

where *itmax* is the number of iterations, prescribed, *eps* is the accuracy desired and $z_{i+1,j}^{(k)}$ (respectively $z_{i+1,j}$) denote the approximated solution for $z_\varepsilon^{(k)}((i+1)\varepsilon)$ (respectively $z_\varepsilon((i+1)\varepsilon)$), $\forall x_j,\ j=\overline{1,N-1}$.

For the numerical tests we consider:

$$T=15.,\quad c=100,\quad \xi=.5,\quad a=\xi^{\frac{1}{4}},\quad l=3.,\quad k=.9,\quad \tau=10^{-2}\cdot\xi^2.$$

$\left(kl^2<16\xi^2/\tau \ \text{ and } \ l>2a\right)$.

The initial value $\varphi_0(x)$ is chosen such that (see Figure 3 for $i=0$)

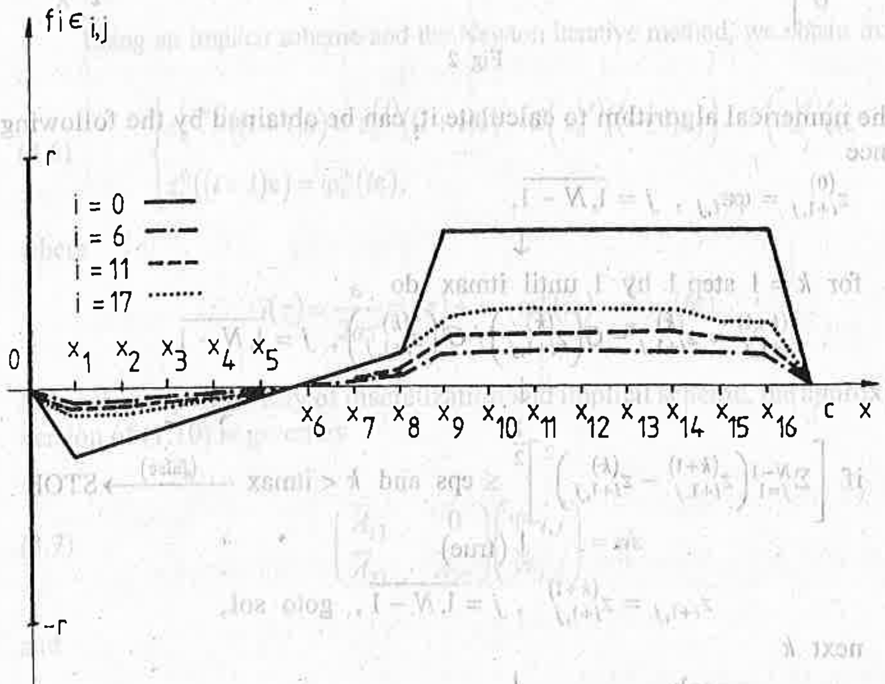


Fig. 3

$$\varphi_0(x_0)=0,\qquad \varphi_0(x_N)=0,$$

$$\varphi_0(x_j)=-0.55+(j-1)/10,\quad j=\overline{1,[N/2]},$$

$$\varphi_0(x_j)=1.1,\quad j=\overline{[N/2]+1,N-1}$$

and the initial value $u_0(x)$ is the solution of stationary equation $\varphi_t=\Delta\varphi=0$, i.e. the solution of the following equation (see Figure 4 for $i=0$)

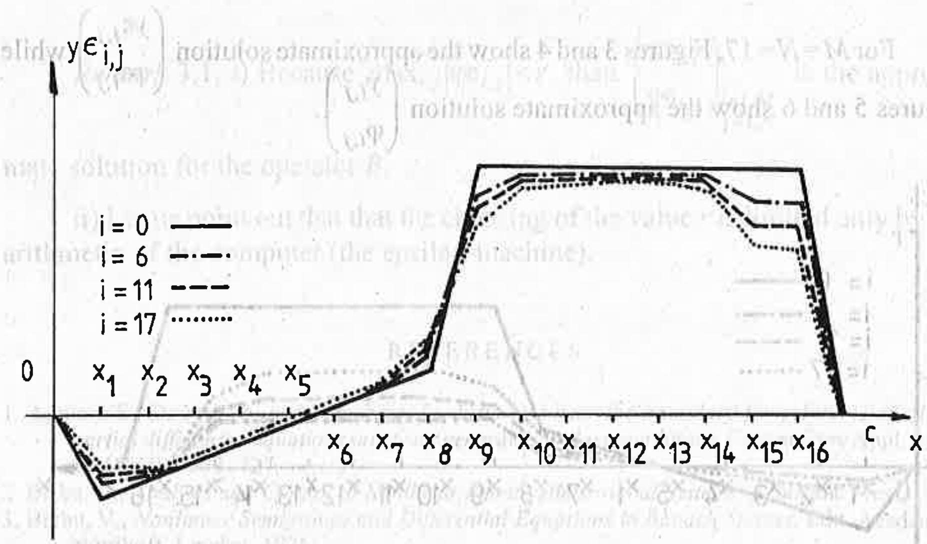


Fig. 4

$$(2a)^{-1}\left(\varphi-\varphi^3\right)+2u=0,$$

(see also [10] or [12]).

We observe that $\max_j\left|\varphi_0(x_j)\right|=1.1$ and thereby if we choose $r=\max_j\left|\varphi_0(x_j)\right|+2$ then $g_r\left(\varphi_0(x_j)\right)=\varphi_0(x_j)^3$, $j=\overline{0,N}$, and then $B_r\begin{pmatrix} y_0(x_j)\\ \varphi_0(x_j)\end{pmatrix}=B\begin{pmatrix} y_0(x_j)\\ \varphi_0(x_j)\end{pmatrix}$.

In Table 1 there are given some numerical tests executed on a PC 386SX computer with math coprocessor.

Table 1

	The CPU-time spent by fractional step method	The CPU-time spent by iterative Newton method (3.5)	M	N
1	83 hund	1" 10 hund	17	17
2	5" 11 hund	7" 42 hund	17	37
3	8" 89 hund	11" 26 hund	27	37
4	11" 37 hund	15" 92 hund	37	37
5	14" 94 hund	20" 05 hund	47	37

For $M=N=17$, Figures 3 and 4 show the approximate solution $\begin{pmatrix} y\varepsilon_{i,j} \\ \varphi\varepsilon_{i,j} \end{pmatrix}$ while Figures 5 and 6 show the approximate solution $\begin{pmatrix} y_{i,j} \\ \varphi_{i,j} \end{pmatrix}$.

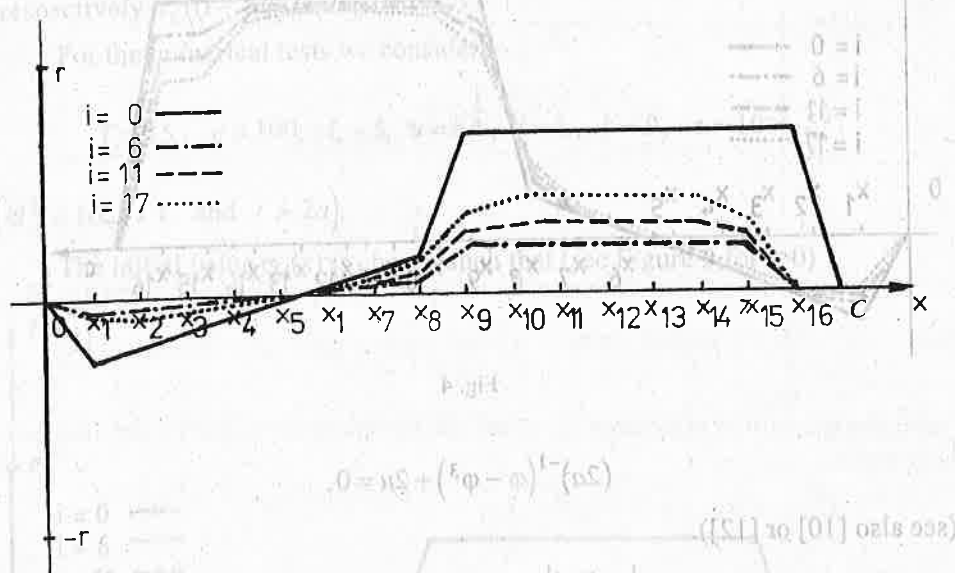


Fig. 5

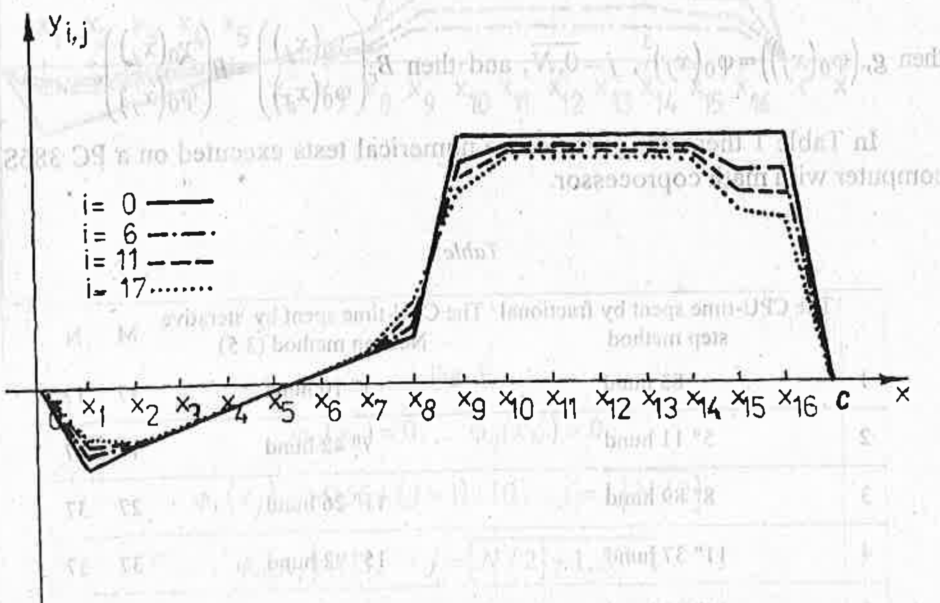


Fig. 6

Remark 3.1. i) Because $\max_{i,j}|\varphi\varepsilon_{i,j}|<r$, then $\begin{pmatrix} y\varepsilon_{i,j} \\ \varphi\varepsilon_{i,j} \end{pmatrix}_{\substack{i=1,M \\ j=1,N}}$ is the approximate solution for the operator B.

ii) Let us point out that that the choosing of the value r is limited only by the arithmetic of the computer (the epsilon-machine).

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