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FULLY DISCRETE FINITE ELEMENT SCHEMES FOR THE CAHN-HILLIARD EQUATION

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Research Report No. 88-34 α

September 1988

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**Proceedings of "International Conference on Numerical Mathematics",
National University of Singapore 31 May - 4 June 1988.**

Introduction

We consider the nonlinear evolution equation

$$(1.1a) \quad u_t + \gamma D^4 u = D^2 \varphi(u), \quad x \in I = (0, L), \quad t > 0$$

with boundary conditions

$$(1.1b) \quad Du = D^3 u = 0 \quad \text{at } x = 0, L$$

and initial condition

$$(1.1c) \quad u(\cdot, 0) = u_0$$

where $D \equiv \frac{\partial}{\partial x}$, γ is a prescribed positive constant and $\varphi \in C^1(\mathbb{R})$ is a prescribed function.

If

$$\varphi(u) = u(u^2 - \beta^2)$$

then (1.1a) is the Cahn-Hilliard equation, see Cahn [1968], Novick-Cohen & Segel [1984], Elliott & French [1987], and the references cited therein.

The Cahn-Hilliard generalized diffusion equation has been proposed to model phase separation in a binary mixture where u is a scaled concentration. The solution $u(x, t)$ exhibits pattern formation with interfaces separating regions where u is nearly constant taking the phase values $\pm \beta$. Also in the time evolution the solution reaches certain states and remains close to them for a long time before evolving into different states of lower energy; this phenomenon is called metastability.

We assume that (1.1) has a unique solution for $t \in [0, T]$. Further we assume that the solution is sufficiently smooth and

$$(1.2) \quad \|u(\cdot, t)\|_{L^\infty(I)} \leq M \quad \forall t \in [0, T].$$

In the case of the Cahn-Hilliard equation global existence and boundedness of u has been proved in Elliott & Zheng [1986].

A weak formulation for this problem is: (P) Find $u(\cdot, t) \in H_E^2(I)$ for $t \in [0, T]$ such that

$$(1.3) \quad (u_t, v) + \gamma(D^2 u, D^2 v) = (\varphi(u), D^2 v) \quad \forall v \in H_E^2(I)$$

with $u(\cdot, 0) = u_0$;

where

$$(v, w) \equiv \int_I v(x)w(x)dx,$$

$$H_E^2(I) = \left\{ v \in H^2(I) : Dv = 0 \quad \text{at } x = 0 \quad \text{and } x = L \right\}.$$

Throughout this note the norms in $L^\infty(I)$, $L^2(I)$ and $H^s(I)$ are denoted by $\|\cdot\|_{0,\infty}$, $\|\cdot\|_0$ and $\|\cdot\|_s$. The semi-norm $|D^s v|_0$ is denoted by $|v|_s$.

Numerical Method: Let S_h^r be the piecewise polynomial spline space

$$S_h^r = \{ \chi \in C^{r-2}(I) : \chi|_{I_j} \in P_{r-1}(I_j), j = 1 \dots N \}$$

where $r \geq 3$ is an integer;

$$0 = x_0 < x_1 < \dots < x_N = L$$

is a partition of $I = (0,L)$ with $I_j = (x_{j-1}, x_j)$, $h = \max_j (x_j - x_{j-1})$ and

$P_{r-1}(I_j)$ denotes the set of all polynomial functions on I_j of degree less than or equal to $r-1$. Define

$$S_h^{0r} = \{ \chi \in S_h^r : D\chi = 0 \text{ at } x = 0 \text{ and } x = L \}$$

and let

$$\alpha \geq h (\min_j (x_j - x_{j-1}))^{-1}$$

where we assume that for a family of partitions α is fixed.

The approximation scheme using a Galerkin method in space and Crank-Nicolson time discretization gives the following problem: $(P_{h,k})$. Find $\{U^n\}_{0 \leq nk \leq T}$ such that $U^n \in S_h^{0r}$,

$$(1.4) \quad (\partial U^n, \chi) + \gamma(D^2 U^{n+1/2}, D^2 \chi) = (\varphi(U^{n+1/2}), D^2 \chi)$$

for all $\chi \in S_h^{0r}$ and $U^0 = u_0^h$;

where u_0^h is an approximation of u_0 ,

$$\partial V^n = \frac{1}{k} (V^{n+1} - V^n)$$

and

$$U^{n+1/2} = \frac{1}{2} (U^{n+1} + U^n).$$

For $v \in H_E^2(I)$, let $P_h v \in S_h^{0r}$ be the unique solution of

$$(D^2 P_h v - D^2 v, D^2 \chi) = 0 \text{ for all } \chi \in S_h^{0r}$$

where $(\chi, 1) = 0$ and $(P_h v, 1) = (v, 1)$. If $\rho^n = P_h u(\cdot, nk) - u(\cdot, nk)$ then

$$(1.5) \quad \left\| \left(\frac{\partial}{\partial t} \right)^j \rho^n \right\|_0 \leq Ch^{\bar{r}}; \quad j = 0, 1; \quad 0 \leq nk \leq T$$

where

$$\bar{r} = \begin{cases} 2 & \text{if } r=3 \\ r & \text{otherwise} \end{cases}$$

and C depends on $\left\| \left(\frac{\partial}{\partial t} \right)^j u \right\|_r$; see Elliott & Zheng [1986].

We will assume that

$$(1.6) \quad |u_0^h - u(\cdot, 0)|_0 \leq Ch^{\bar{r}}$$

where C is independent of h, k .

We also need the subspace inequality

$$(1.7) \quad |\chi|_{0,\infty} \leq \frac{C}{h} |\chi|_0 \quad \forall \chi \in S_h^{0,r}$$

where C depends on r and α .

Error bounds for the continuous in time Galerkin approximation of the Cahn-Hilliard equation based on the spaces $S_h^{0,r}$ were obtained in Elliott & Zheng [1986]. Numerical experiments based on the Crank-Nicolson time discretization (1.4) are reported on in Elliott & French [1987]. Also in this latter paper an error analysis was carried out based on the assumptions that (A) (1.4) has a unique solution for k sufficiently small and (B) $|U^n|_{0,\infty}$ is uniformly bounded independently of h and k . It is the purpose of this note to justify (B) and to show that (1.4) has a unique solution in the ball $B = \{\chi \in S_r^{0,h} : |\chi|_{0,\infty} \leq M+1\}$ for h and k sufficiently small. We also analyse an iterative method to solve (1.4) which is similar but slightly different to that used in Elliott & French [1987].

Section 3 has the main Theorem of this note which is an optimal order error estimate for the fully discrete Crank-Nicolson method (1.4) where the solution is obtained at each time step by a fixed point iteration procedure. Section 2 has several auxiliary results for (1.1) in the special case where φ' is bounded. The main idea here is that because we are interested in computing with unbounded φ' the error analysis of (1.4) requires an L^∞ bound on U^n . Unfortunately it is not clear how to obtain an a priori bound simply by studying (1.4). However since (1.4) is a perturbation of (1.1), it is possible to use the boundedness of $u(x,t)$ to derive the fact that there is a unique solution $U^n \in B$ for h and k sufficiently small.

2. Bounded $\varphi'(\cdot)$

In this section we study the fully discrete approximation of (1.1) under the assumption that φ' is bounded. These results are used in section 3 in the analysis of the interesting case of (1.4) with φ' unbounded.

Proposition 2.1. Let $\varphi(\cdot)$ be such that

$$(2.1) \quad \varphi \in C^1(\mathbb{R}) \quad ; \quad \sup_{s \in \mathbb{R}} |\varphi'(s)| \leq \lambda$$

There exists a $k_0 > 0$, sufficiently small such that for

$$(2.2) \quad k < k_0$$

there is a unique sequence $\{U^n\}_{0 \leq nk \leq T}$ solving (1.4) and

$$(2.3) \quad |U^n - u(\cdot, nk)|_0 \leq C(u) (h^{\bar{r}} + k^2)$$

$$(2.4) \quad |U^n - u(\cdot, nk)|_{0, \infty} \leq C(u)(h^{\bar{r}-1} + k^2/h).$$

Furthermore for each $n > 0$ and $U_0^n \in \mathring{S}_h^r$ the sequence $\{U_j^n\}_{j=0}^\infty$ defined by:

$$(2.5) \quad (U_j^n, \chi) + \frac{\gamma k}{2} (D^2 U_j^n, D^2 \chi) = k(\varphi(\frac{1}{2}(U_{j-1}^n + U^{n-1})), D^2 \chi) + (U^{n-1}, \chi) \\ - \frac{\gamma k}{2} (D^2 U^{n-1}, D^2 \chi) \quad \forall \chi \in \mathring{S}_h^r$$

converges to U^n at the rate.

$$(2.6) \quad |U_j^n - U^n|_0^2 \leq \left(k \frac{\lambda^2}{4\gamma}\right)^j |U_0^n - U^n|_0^2$$

and

$$(2.7) \quad |U_j^n - U^n|_{0, \infty}^2 \leq C \frac{\lambda}{\gamma} \left(k \frac{\lambda^2}{4\gamma}\right)^{j-1/2} |U_0^n - U^n|_0^2.$$

Proof: For fixed $n \geq 1$, given $U_0^n \in \mathring{S}_h^r$ it is clear that (2.5) generates a well defined sequence $\{U_j^n\}$ since the bilinear form $(\cdot, \cdot) + \frac{\gamma k}{2} (D^2 \cdot, D^2 \cdot)$ is strictly coercive on \mathring{S}_h^r . Set $e_j = U_{j+1}^n - U_j^n$. It follows by subtraction that for each $\chi \in \mathring{S}_h^r$ we have

$$(2.8) \quad (e_j, \chi) + \frac{k\gamma}{2} (D^2 e_j, D^2 \chi) = k([\varphi(\frac{1}{2}(U_j^n + U^{n-1})) - \varphi(\frac{1}{2}(U_{j-1}^n + U^{n-1}))], D^2 \chi)$$

Taking $\chi = e_j$ in (2.8) yields

$$\begin{aligned} |e_j|_0^2 + \frac{\gamma k}{2} |e_j|_2^2 &= \frac{k}{2} (\varphi'(\eta_j^n) e_{j-1}, D^2 e_j) \\ &\leq \frac{k\lambda}{2} |e_{j-1}|_0 |e_j|_2 \\ &\leq \frac{k}{2} \left[\frac{\lambda^2}{2\gamma} |e_{j-1}|_0^2 + \frac{\gamma}{2} |e_j|_2^2 \right] \end{aligned}$$

so that

$$(2.9a) \quad |e_j|_0^2 + \frac{\gamma k}{4} |e_j|_2^2 \leq \frac{k\lambda^2}{4\gamma} |e_{j-1}|_0^2$$

$$(2.9b) \quad |e_j|_0^2 \leq \left(\frac{k\lambda^2}{4\gamma} \right)^j |e_0|_0^2$$

Taking k sufficiently small, $\{U^n\}$ is a Cauchy sequence with limit $U^n \in \mathcal{S}_h^0$ and, by the continuity of φ , passing to the limit in (2.5) yields (1.4). A similar argument yields the uniqueness of U^n solving (1.4). Furthermore setting $E_j = U_j^n - U^n$ and subtracting (1.4) from (2.5) we obtain the following analogue of (2.9)

$$(2.10a) \quad |E_j|_0^2 + \frac{\gamma k}{4} |E_j|_2^2 \leq \frac{k\lambda^2}{4\gamma} |E_{j-1}|_0^2$$

$$(2.10b) \quad |E_j|_0^2 \leq \left(\frac{k\lambda^2}{4\gamma} \right)^j |E_0|_0^2$$

Note that (2.10b) proves (2.6).

In order to prove (2.7) note that taking $\chi=1$ in (1.4) and (2.5) yields $(E_j, 1) = 0$ so that by the Poincaré inequality

$$|v|_0 \leq C (|v|_1 + |(v, 1)|) \quad \forall v \in H^1(\Omega),$$

the inequality

$$|v|_1 \leq |v|_2^{1/2} |v|_0^{1/2} \quad \forall v \in H_E^2(\Omega),$$

and the Sobolev inequality

$$|v|_{0,\infty} \leq C \|v\|_1 \quad \forall v \in H^1(\Omega)$$

we obtain

$$|E_j|_{0,\infty} \leq C |E_j|_0^{1/2} |E_j|_2^{1/2};$$

applying (2.10) yields (2.7).

We now turn to the proof of (2.3) and (2.4). To prove (2.3) we use standard techniques (see Thomeé [1984]). For completeness, parts of the proof from Elliott

& French [1987] are included below.

Let $t_n = nk$, $P_h u^n \equiv P_h^n(u, t_n)$ and $t_{n+1/2} = \frac{1}{2}(t_n + t_{n+1})$.

We use the standard error decomposition:

$$U^n - u(\cdot, t_n) = [U^n - P_h u^n] + [P_h u^n - u(\cdot, t_n)] = \theta^n + \rho^n$$

Using (1.4) we have

$$\begin{aligned} (\partial \theta^n, \chi) + \gamma(D^2 \theta^{n+1/2}, D^2 \chi) &= (\varphi(U^{n+1/2}) - \varphi(u(\cdot, t_{n+1/2})), D^2 \chi) \\ &\quad - (\partial P_h u^n - u_t, \chi) - \gamma(D^2 [\frac{1}{2}u(\cdot, t_{n+1}) + \frac{1}{2}u(\cdot, t_n) - u(\cdot, t_{n+1/2})], D^2 \chi). \end{aligned}$$

Setting $\chi = \theta^{n+1/2}$, the above becomes

$$(2.11) \quad (\partial \theta^n, \theta^{n+1/2}) + \gamma |\theta^{n+1/2}|_2^2 \leq [|\varphi(U^{n+1/2}) - \varphi(u(\cdot, t_{n+1/2}))|_0 +$$

$$|\partial P_h u^n - u_t(\cdot, t_{n+1/2})|_0 + \gamma |\frac{1}{2}u(\cdot, t_{n+1}) + \frac{1}{2}u(\cdot, t_n) - u(\cdot, t_{n+1/2})|_2] |\theta^{n+1/2}|_2$$

Using the Cauchy-Schwarz inequality, we obtain

$$(2.12) \quad (\partial \theta^n, \theta^{n+1/2}) \leq C(I_1 + I_2 + I_3)^2,$$

where the I 's are the three terms in the first factor on the right-hand side of

(2.11). Estimate I_3 :

$$\begin{aligned} I_3 &= \gamma \left| \int_{t_{n+1/2}}^{t_{n+1}} (s - t_{n+1/2}) u_{tt}(\cdot, s) ds - \int_{t_n}^{t_{n+1/2}} (s - t_{n+1/2}) u_{tt}(\cdot, s) ds \right|_0^2 \\ &\leq \gamma k^{\frac{3}{2}} \left(\int_{t_n}^{t_{n+1}} \|u_{tt}(\cdot, s)\|_2^2 ds \right). \end{aligned}$$

Estimate I_1 :

$$\begin{aligned} I_1 &= |\varphi'(\eta)[U^{n+1/2} - u(\cdot, t_{n+1/2})]|_0 \leq \lambda |U^{n+1/2} - u(\cdot, t_{n+1/2})|_0, \\ &\leq C[|\theta^{n+1/2}|_0 + \frac{1}{2}(|\rho^{n+1}|_0 + |\rho^n|_0) + \frac{1}{2}u(\cdot, t_{n+1}) + \frac{1}{2}u(\cdot, t_n) - u(\cdot, t_{n+1/2})|_0]. \end{aligned}$$

The last term in the above is estimated in the same way as I_3 .

Finally we consider I_2 . Let $\partial u(\cdot, t_n) = k^{-1}(u(\cdot, t_{n+1}) - u(\cdot, t_n))$.

$$\begin{aligned}
I_2 &\leq |\partial P_h u^n - \partial u(\cdot, t_n)|_0 + |\partial u(\cdot, t_n) - u_t(\cdot, t_{n+1/2})|_0 \\
&= k^{-1} |\rho^{n+1} - \rho^n|_0 + |k^{-1}(u(\cdot, t_{n+1}) - u(\cdot, t_n)) - u_t(\cdot, t_{n+1/2})|_0 \\
&\leq k^{-1/2} \left(\int_{t_n}^{t_{n+1}} |\rho_t(\cdot, s)|_0^2 ds \right)^{1/2} \\
&\quad + k^{-1} \left(\left| \int_{t_{n+1/2}}^{t_{n+1}} (s - t_{n+1/2})^2 u_{ttt}(\cdot, s) ds - \int_{t_n}^{t_{n+1/2}} (s - t_{n+1/2})^2 u_{ttt}(\cdot, s) ds \right|_0 \right) \\
&\leq k^{-1/2} \left(\int_{t_n}^{t_{n+1}} |\rho_t(\cdot, s)|_0^2 ds \right)^{1/2} + k^{3/2} \left(\int_{t_n}^{t_{n+1}} |u_{ttt}(\cdot, s)|_0^2 ds \right)^{1/2}
\end{aligned}$$

With these estimates (2.12) becomes

$$\frac{1}{2} k^{-1} (|\theta^{n+1}|_0^2 - |\theta^n|_0^2) \leq C (|\theta^{n+1/2}|_0^2 + w_n),$$

where

$$w_n = |\rho^{n+1}|_0^2 + |\rho^n|_0^2 + k^3 \left(\int_{t_n}^{t_{n+1}} \|u_{tt}(\cdot, s)\|_2^2 + |u_{ttt}(\cdot, s)|_0^2 ds \right) + k^{-1} \int_{t_n}^{t_{n+1}} |\rho_t(\cdot, s)|_0^2 ds,$$

which yields

$$|\theta^{n+1}|_0^2 \leq \frac{1 + Ck}{1 - Ck} |\theta^n|_0^2 + Ckw_n.$$

Iterating this inequality, we have for $k_0 < 1/2 C$

$$|\theta^n|_0^2 \leq C(T) \left(|\theta^n|_0^2 + Ck \sum_{j=0}^{n-1} w_j \right).$$

Noting that

$$|\theta^0|_0^2 \leq |\rho^0|_0^2 + |U^0 - u_0|_0^2.$$

we obtain (2.3) by recalling the bounds (1.5).

It remains to prove (2.4). We note that there exists

$I_h u(\cdot, t_n) \in \mathcal{S}_h^r$, an interpolant of $u(\cdot, t_n)$, which satisfies

$$|I_h u(\cdot, t_n) - u(\cdot, t_n)|_{0,\infty} \leq C(u) h^r$$

so that, using the inverse norm inequality (1.7),

$$\begin{aligned}
|U^n - u(\cdot, t_n)|_{0,\infty} &\leq C(u) h^r + |I_h u(\cdot, t_n) - U^n|_{0,\infty} \\
&\leq C(u) h^r + Ch^{-1} |I_h u(\cdot, t_n) - U^n|_0 \\
&\leq C(u) h^r + Ch^{-1} [|I_h u(\cdot, t_n) - u(\cdot, t_n)|_0 \\
&\quad + |u(\cdot, t_n) - U^n|_0]
\end{aligned}$$

and so (2.4) now follows from (2.3).

Corollary 2.1: There exists constants $h_0 > 0$ and $\varepsilon_0 > 0$ independent of h and k such that if $h \leq h_0$, $k^2/h \leq \varepsilon_0$ and

$$(2.13) \quad |U_0^n|_{0,\infty} \leq K \quad \text{for } 0 \leq nk \leq T$$

for some constant $K > 0$ then

$$|U_j^n|_{0,\infty} \leq M + 1 \quad \text{for } 0 \leq nk \leq T$$

and $j = 1, 2, \dots$.

Proof:

From the estimate (2.4) and the given bound (1.2) on u we have

$$|U^n|_{0,\infty} \leq M + C(u) (h^{\bar{r}-1} + \frac{k^2}{h}) .$$

(2.7) gives

$$\begin{aligned} |U_j^n|_{0,\infty} &\leq |U^n|_{0,\infty} + (ck)^{1/2} |U_0^n - U^n|_0 \\ &\leq (1 + (ck)^{1/2}) |U^n|_{0,\infty} + (ck)^{1/2} |U_0^n|_{0,\infty} \\ &\leq (M + C(u) (h^{\bar{r}-1} + \frac{k^2}{h})) (1 + (ck)^{1/2}) + (ck)^{1/2} K. \end{aligned}$$

Clearly for ε_0 and h_0 sufficiently small the right hand side is less than $M + 1$.

3 Unbounded $\varphi'(\cdot)$

We now consider (1.1) and (1.4) without requiring that $\varphi'(\cdot)$ be bounded; this is the case for the Cahn-Hilliard equation where

$$\varphi(u) = 3u^2 - \beta^2.$$

In order to obtain error bounds for this case we analyse problem $(\tilde{P}_{h,k}^{\tilde{\varphi}})$ which has φ replaced by $\tilde{\varphi} \in C^1(\mathbb{R})$ such that

$$(3.1a) \quad \tilde{\varphi}(s) = \varphi(s) \quad \text{for } |s| \leq M+1$$

and

$$(3.1b) \quad \sup_{s \in \mathbb{R}} |\tilde{\varphi}'(s)| \leq \lambda$$

In this case we know that, because of the assumptions (1.2), the initial boundary-value problem (1.1) has the same unique solution when φ is replaced by $\tilde{\varphi}$.

Theorem 3.1: There exist positive constants h_0 and ε_0 such that for $h \leq h_0$ and $k^2 \leq \varepsilon_0 h$:

(i) (1.4) has a unique solution U_B^n in the ball

$$B = \left\{ \chi \in S_h^r : |\chi|_{0,\infty} \leq M+1 \right\}.$$

(ii) For every $U_0^n \in B$ the fixed point iteration (2.5) converges to U_B^n .

(iii) The error bound

$$|U_B^n - u(\cdot, t_n)| \leq C(u) (h^{\bar{r}} + k^2)$$

holds.

Proof: Let U^n and U_j^n denote solutions of $(\tilde{P}_{n,k})$ and (2.5) for fixed n with φ replaced by $\tilde{\varphi}$. Proposition 2.1 applies and we know that \tilde{U}^n is unique and is the limit as $j \rightarrow \infty$ of the well defined sequence $\{\tilde{U}_j^n\}$. Furthermore it follows from the Proposition and Corollary 2.1 that $U^n \in B$ and $\tilde{U}_j^n \in B$ for each $n \geq 1$ and $j = 0, 1, 2, \dots$. Since φ is identical to $\tilde{\varphi}$ on the ball B , Theorem 3.1 is an immediate consequence of section 2 with

$$U_j^n = \tilde{U}_j^n, \quad U_B^n = \tilde{U}^n.$$

Remark: Suitable choices for $U_0^n \in B$ are

$$a) \quad U_0^n = U^{n-1} \quad b) \quad U_0^n = 2U^{n-1} - U^{n-2}.$$

In case b) the fact that $U_0^n \in B$ is a consequence of the fact that $2U^{n-1} - U^{n-2}$ approximates $2u(\cdot, t_{n-1}) - u(\cdot, t_{n-2})$ in L^∞ and the latter approximates $u(\cdot, t_n)$ to order k^2 .

Remark: We considered other fully discrete numerical methods for problem (1.1). The backward Euler method for (1.1), "time-lagging" the nonlinear term, is given by the problem: Find $\{U^n\}_{0 \leq nk \leq T}$ such that $U^n \in \tilde{S}_h^r$

$$(3.2) \quad (\partial U^n, \chi) + \gamma (D^2 U^{n+1}, D^2 \chi) = (\varphi(U^n), D^2 \chi)$$

for all $\chi \in \tilde{S}_h^r$ and $U_0^0 = U_0^h$. An optimal order linearized

Crank-Nicholson method is defined as above with (3.2) replaced by the expression below

$$(3.3) \quad (\partial U^n, \chi) + \gamma (D^2 U^{n+1/2}, D^2 \chi) = (\varphi(\frac{3}{2} U^n - \frac{1}{2} U^{n-1}), D^2 \chi).$$

Again the nonlinear term is "time lagged". A Crank-Nicholson predictor-corrector method has two steps. The prediction function is found by (3.3). Labelling this solution W^{n+1} the correction function is found by the expression

$$(3.4) \quad (\partial U^n, \chi) + \gamma (D^2 U^{n+1/2}, D^2 \chi) = \left(\varphi \left(\frac{1}{2} (W^{n+1} + U^n) \right), D^2 \chi \right)$$

as above.

On each time step all the methods discussed above define a unique selection U^{n+1} given U^n . We can prove there exist constants C, ϵ_0 and h_0 such that

(i) If $\{U^n\}$ is given by the backward Euler method (3.2), $h \leq h_0$ and $k \leq \epsilon_0 h$ then

$$(3.5) \quad |U - u(\cdot, t_n)|_0 \leq C (h^{\bar{r}} + k)$$

(ii) If $\{U^n\}$ is given by either of the Crank-Nicholson methods, $h \leq h_0$ and $k \leq \sqrt{\epsilon_0 h}$ then

$$(3.6) \quad |U^n - u(\cdot, t_n)|_0 \leq C (h^{\bar{r}} + k^2)$$

Acknowledgement : We thank L.B. Wahlbin and R.A. Nicolaides for helpful conversations.

This work was partially supported by the National Science Foundation, Grant No: DMS - 8802828.

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