A penalty approach to the numerical simulation of a constrained wave motion.

R. GLOWINSKI *, A. LAPIN †, and S. LAPIN‡

26th October 2003

Abstract — The main goal of this article is to investigate the numerical solution of a vector-valued nonlinear wave equation, the nonlinearity being of the Ginzburg-Landau type, namely \( (|\vec{u}|^2 - 1)\dot{\vec{u}} \). This equation is obtained when treating by penalty a constrained wave-motion, where the displacement vector is of constant length (1 here, after rescaling). An important step of the approximation process is the construction of a time discretization scheme preserving - in some sense - the energy conservation property of the continuous model. The stability properties of the above scheme are discussed. The authors discuss also the finite element approximation and the quasi-Newton solution of the nonlinear elliptic system obtained at each time step from the time discretization. The results of numerical experiments are presented; they show that for the constraint of the original wave problem to be accurately verified we need to use a small value of the penalty parameter.

1. INTRODUCTION

The main goal of this paper is to address the solution of a constrained wave system which has application in theoretical and applied physics. The numerical methodology relies on: the penalty treatment of the constraint and an energy preserving time discretization leading to a scheme which is essentially unconditionally stable and second order accurate, both techniques being combined with a globally continuous piecewise linear finite element approximation. The results of numerical experiments illustrate the properties of the computational methods discussed here, particularly energy and length preservation.

2. DIFFERENTIAL PROBLEM

Let \( \Omega \) be a bounded domain in \( R^2 \) with a piecewise smooth boundary \( \partial \Omega \) and let \( \vec{u}(x,t) : \Omega \times (0,T) \to R^3 \). We consider the following constrained wave problem

\[
\frac{\partial^2 \vec{u}}{\partial t^2} - \Delta \vec{u} + \lambda \vec{u} = 0, \quad |\vec{u}|^2 = 1 \quad \text{in } \Omega \times (0,T)
\]  

*(University of Houston, Houston, TX, 77204, USA)
†Kazan State University, Kazan, 420008, Russia
‡University of Houston, Houston, TX, 77204, USA
with Dirichlet boundary conditions
\[ \tilde{u}(x,t) = \tilde{g}(x, t) \text{ on } \partial \Omega \times (0, T), \]
(2.2)
and initial conditions
\[ \tilde{u}(x, 0) = \tilde{u}_0(x), \quad \frac{\partial \tilde{u}}{\partial t}(x, 0) = \tilde{u}_1. \]
(2.3)
Further we suppose that \( \tilde{g} = \tilde{g}(x) \) and
\[ \left\{ \begin{array}{ll}
\tilde{u}_0(x) \cdot \tilde{u}_1(x) = 0, & |\tilde{u}_0(x)|^2 = 1 \quad \text{for a.a. } x \in \Omega, \\
|\tilde{g}(x)|^2 = 1 & \text{for a.a. } x \in \partial \Omega.
\end{array} \right. \]
(2.4)

**Remark 2.1.** Function \( \lambda \) is clearly a Lagrange multiplier associated to the constraint \( |\tilde{u}|^2 = 1 \).

We approximate the constrained wave equation (2.1) by the following wave equation with penalty term:
\[ \frac{\partial^2 \tilde{u}}{\partial t^2} - \Delta \tilde{u} + \frac{1}{\varepsilon}(|\tilde{u}|^2 - 1)\tilde{u} = 0, \]
(2.5)
namely a kind of "Ginzburg-Landau wave equation" (for more information on Ginzburg-Landau type models see, e.g., [1]).

Using the methods from [5] we can prove the following

**Proposition 2.1.** For every fixed \( \varepsilon > 0 \) problem (2.2) – (2.5) has a unique solution such that \( \tilde{u} \in L^\infty(0, T; H^1(\Omega)^3), \frac{\partial \tilde{u}}{\partial t} \in L^\infty(0, T; L^2(\Omega)^3) \), provided that \( \tilde{u}_0 \in H^1(\Omega)^3, \tilde{u}_1 \in L^2(\Omega)^3, \tilde{g} \in H^{1/2}(\partial \Omega)^3 \) and assumptions (2.4) are fulfilled.

We show that model (2.2) – (2.5) is energy preserving. Multiplying (2.5) by \( \frac{\partial \tilde{u}}{\partial t} \) and integrating over \( \Omega \) we obtain:
\[ \frac{1}{2} \frac{d}{dt} \int_\Omega |\frac{\partial \tilde{u}}{\partial t}|^2 dx + \frac{1}{2} \frac{d}{dt} \int_\Omega |\nabla \tilde{u}|^2 dx + \frac{1}{4\varepsilon} \frac{d}{dt} \int_\Omega (|\tilde{u}|^2 - 1)^2 dx = 0, \]
which implies that the energy
\[ E_\varepsilon(t) = \frac{1}{2} \int_\Omega |\frac{\partial \tilde{u}(t)}{\partial t}|^2 dx + \frac{1}{2} \int_\Omega |\nabla \tilde{u}(t)|^2 dx + \frac{1}{4\varepsilon} \int_\Omega (|\tilde{u}(t)|^2 - 1)^2 dx \]
of the system is constant in time. Above, we have denoted by \( \tilde{u}(t) \) the function \( x \to \tilde{u}(x,t) \). Due to assumption \( |\tilde{u}_0(x)|^2 = 1 \) the energy \( E(0) \) doesn’t depend upon
the penalty parameter $\varepsilon$ and reduces to

$$E(0) = \frac{1}{2} \left( \int_{\Omega} |\tilde{u}_1|^2 dx + \int_{\Omega} |\nabla \tilde{u}_0|^2 dx \right).$$

This equality and the energy conservation imply the following estimate for any $t > 0$

$$\int_{\Omega} (|\tilde{u}|^2 - 1)^2 dx \leq 2\varepsilon \left( \int_{\Omega} |\tilde{u}_1|^2 dx + \int_{\Omega} |\nabla \tilde{u}_0|^2 dx \right). \quad (2.6)$$

3. DISCRETE PROBLEMS

First, we construct a semidiscrete problem by approximating the time derivative in equation (2.5). Let $\Delta t > 0$ be a time step and set $u^n \approx u(n\Delta t)$ for $n = 1, 2, \ldots$. Then, we consider the following time discretization scheme:

$$\frac{\tilde{u}^{n+1} + \tilde{u}^{n-1} - 2\tilde{u}^n}{\Delta t^2} - \Delta \left( \frac{\tilde{u}^{n+1} + 2\tilde{u}^n + \tilde{u}^{n-1}}{4} \right) + \frac{1}{2\varepsilon} \left( \left( \frac{\tilde{u}^n + \tilde{u}^{n+1}}{2} \right)^2 + \left( \frac{\tilde{u}^n + \tilde{u}^{n-1}}{2} \right)^2 - 2 \right) \left( \frac{\tilde{u}^{n+1} + 2\tilde{u}^n + \tilde{u}^{n-1}}{4} \right) = 0, \quad (3.1)$$

with corresponding boundary conditions. Scheme (3.1) is initialized with

$$\begin{cases} 
\tilde{u}^0 = \tilde{u}_0, \quad \tilde{u}^1 - \tilde{u}^{-1} = 2\Delta t \tilde{u}_1, \\
\tilde{u}^1 - 2\tilde{u}^0 + \tilde{u}^{-1} = \Delta t^2 \Delta \tilde{u}^0.
\end{cases} \quad (3.2)$$

The semidiscrete problem keeps (in some sense) the energy preserving property of the initial problem. Approximate energy $E_\varepsilon$ at $t = (n + 1/2)\Delta t$ by

$$E_\varepsilon^{n+1/2} = \frac{1}{2} \int_{\Omega} \frac{\tilde{u}^{n+1} - \tilde{u}^n}{\Delta t}^2 dx + \frac{1}{2} \int_{\Omega} \frac{|\nabla \tilde{u}^{n+1} + \tilde{u}^n|}{2}^2 dx$$

$$+ \frac{1}{4\varepsilon} \int_{\Omega} \left( \frac{\tilde{u}^{n+1} + \tilde{u}^n}{2} - 1 \right)^2 dx; \quad (3.3)$$

multiplying (3.1) by $(\tilde{u}^{n+1} - \tilde{u}^{n-1})/2$ and integrating in $x$ over $\Omega$ we obtain

$$E_\varepsilon^{n+1/2} = E_\varepsilon^{n-1/2} \forall n. \quad (3.4)$$

The basis of the previous formal calculations will be shown below, when the existence of a weak solution to problem (3.1), (3.2) and its corresponding regularity will be proved.
We construct a finite dimensional approximation of the semidiscrete scheme (3.1) via the finite element method; the simplest quadrature formulae (based on the trapezoidal rule) are used to avoid non-diagonal mass matrices.

Let \( \mathcal{T}_h \) be a regular triangulation of \( \Omega \), that we assume to be polygonal. For simplicity we denote by \( e \) the generic element of triangulation \( \mathcal{T}_h \). By \( V_h \subset (H^1(\Omega))^3 \) we denote the finite element space: \( \{ \bar{v}_h = (v_{1h}, v_{2h}, v_{3h}) \}, v_{ih} \in C^0(\Omega), v_{ih}|_e \in P_1(e) \) for all \( i \) and for all \( e \in \mathcal{T}_h \). For simplicity, let function \( g(x) \) be continuous, i.e. \( g(x) \in (H^{1/2}(\partial \Omega) \cap C^0(\partial \Omega))^3 \) and let \( \bar{g}_h \) be its piecewise linear interpolate: \( \bar{g}_h(x) = g(x) \) at the boundary vertices. We introduce the space \( V^0_h = \{ \bar{v}_h \in V_h : \bar{v}_h = \bar{g}_h \text{ on } \partial \Omega \} \) and test function space \( V^0 = (H^1_0(\Omega))^3 \cap V_h \). Further \( \{ a_i \}^3_{i=1} \) will be the vertices of an element \( e \in \mathcal{T}_h \) of measure \( |e| \). For any function \( \varphi(x) \in C^0(\bar{e}) \), we use the quadrature formulae

\[
\int_e \varphi(x) dx \approx S_e(\varphi) = \frac{1}{3} |e| \sum_{i=1}^{3} \varphi(a_i).
\]

For a function \( \varphi \in C^0(\bar{\Omega}) \) we use \( S_h(\varphi) = \sum_{e \in \Omega} S_e(\varphi) \).

Now a discretization scheme for problem (2.5),(2.2),(2.3) can be written as follows: find \( \bar{u}^n_h \in V^0_h \), such that for all \( \bar{v}_h \in V^0_h \) and all \( n = 1, 2, \ldots \)

\[
S_h(\bar{u}^{n+1}_h - \bar{u}^n_h - 2 \bar{u}^n_h + \bar{v}_h) + \int_{\Omega} \nabla \bar{u}^{n+1}_h + 2 \bar{u}^n_h + \bar{u}^{n-1}_h : \nabla \bar{v}_h dx + \
\frac{1}{2 \varepsilon} S_h((\bar{u}^{n+1}_h + \bar{u}^n_h)^2 + (\bar{u}^n_h + \bar{u}^{n-1}_h)^2 - 2)((\bar{u}^{n+1}_h + 2 \bar{u}^n_h + \bar{u}^{n-1}_h) \cdot \bar{v}_h) = 0,
\]

with the discrete analogue of (3.2):

\[
\begin{cases}
\bar{u}^0_h = \bar{u}_{0h}, \\
S_h(\bar{u}^n_h \cdot \bar{v}_h) = S_h((\bar{u}_{0h} + \Delta t \bar{u}_{1h}) \cdot \bar{v}_h) \\
- \frac{\Delta t^2}{2} \int_{\Omega} \nabla \bar{u}_{0h} : \nabla \bar{v}_h dx, \quad \forall \bar{v}_h \in V^0_h.
\end{cases}
\]

Here, \( \bar{u}_{0h} \in V^0_h \) and \( \bar{u}_{1h} \in V^0_h \) approximate in some sense \( \bar{u}_0 \) and \( \bar{u}_1 \), respectively.

**Remark 3.1.** Higher order finite element methods can be also employed; the technique discussed below would still apply.

The fully discrete scheme (3.5), (3.6) inherits the energy preserving property of the continuous and semidiscrete problems: if the discrete energy is defined by

\[
E^{n+1/2}_h = \frac{1}{2} S_h((\bar{u}^{n+1}_h - \bar{u}^n_h)^2) + \frac{1}{2} \int_{\Omega} |(\bar{u}^{n+1}_h + \bar{u}^n_h)|^2 dx
\]
There exists a definite problem (3.5) in the form

\[ E_h^{n+1/2} = E_h^{1/2} \]  

(3.8)

for all \( n \geq 1 \). To prove it, take \( \tilde{v}_h = \frac{1}{2}(\tilde{u}_h^{n+1} - \tilde{u}_h^{n-1}) \in V_h^0 \) in (3.5).

**Proposition 3.1.** 1) The fully discrete problem (3.5) has a solution for any \( h, \Delta t \) and \( \varepsilon > 0 \).

2) If \( \tilde{u}_1 \in L_p(\Omega)^3 \) and \( \Delta \tilde{u}_0 \in L_p(\Omega)^3 \) for a \( p > 2 \), and \( \Delta t \leq 2\sqrt{\varepsilon} \), then the semidiscrete problem (3.1) has a solution, such that \( \tilde{u}^n \in L_p(\Omega)^3 \) and \( \frac{\tilde{u}^{n+1} + 2\tilde{u}^n + \tilde{u}^{n-1}}{4} \in H^1(\Omega)^3 \) for \( n = 1, 2, \ldots \).

3) If \( \tilde{u} \in H^1(\Omega)^3 \) and \( \Delta \tilde{u}_0 \in H^1(\Omega)^3 \), then problem (3.1) has a solution, such that \( \tilde{u}^n \in H^1(\Omega)^3 \) for all \( n = 1, 2, \ldots \).

**Proof.** 1) To prove the existence of the solution for the fully discrete problem (3.5) we use the following variant of Brouwer theorem [5]:

Let \( V \) be a finite dimensional space endowed with an inner product \((\cdot, \cdot)\) and norm \( ||\cdot||\). Let \( P : V \rightarrow V \) be a continuous mapping with the following property: there exists \( \rho > 0 \) such that \( (P\xi, \xi) \geq 0 \) on the sphere \( ||\xi|| = \rho \). Then there exists a vector \( \xi^* \), \( ||\xi^*|| \leq \rho \) such that \( P\xi^* = 0 \).

We equip the space \( V_h^0 \) with the inner product \((\tilde{v}_h, \tilde{w}_h)_h = S_h(\tilde{v}_h \cdot \tilde{w}_h) \) and the corresponding norm \( ||\tilde{v}_h||_h = S_h^{1/2}(\tilde{v}_h \cdot \tilde{v}_h) \). Let for a fixed \( n \geq 1 \) \( \tilde{v}_h = \frac{1}{2}(\tilde{u}_h^{n+1} - \tilde{u}_h^{n-1}) \in V_h^0 \) and operator \( P : V_h^0 \rightarrow V_h^0 \) be defined by the lefthandside of (3.5). In other words, we write (3.5) in the form \((P\tilde{v}_h, \tilde{v}_h)_h = 0 \ \forall \tilde{v}_h \in V_h^0 \). Operator \( P \) is obviously continuous. Now, if we take \( \tilde{v}_h = \tilde{\tilde{v}}_h \) in (3.5), then

\[ (P\tilde{v}_h, \tilde{v}_h)_h = E_h^{n+1/2} - E_h^{n-1/2} \]  

(3.9)

and it becomes easy to prove that

\[ (P\tilde{v}_h, \tilde{v}_h)_h \geq \frac{1}{2}S_h(\tilde{v}_h \cdot \tilde{v}_h) - c_n \]

with \( c_n \) depending on \( \tilde{u}_h^n \) and \( \tilde{u}_h^{n-1} \) (we recall that \( \tilde{u}_h^n \) and \( \tilde{u}_h^{n-1} \) are supposed to be known). Hence, for \( ||\tilde{v}_h||_h \) large enough we have \((P\tilde{v}_h, \tilde{v}_h)_h \geq 0 \), implying that problem (3.5) has a solution from the above variant of Brouwer theorem.

2) Now we study the solvability of the semidiscrete problem (3.1), using the limit as \( h \rightarrow 0 \) in the fully discrete problem (3.5). Let us introduce, for \( n \geq 1 \) fixed, \( \tilde{v}_i^n = 1/4(\tilde{u}_h^{n+1} + 2\tilde{u}_h^n + \tilde{u}_h^{n-1}) \). We then have the following weak formulation of problem (3.1): find \( \tilde{u}_h^n \in L_p(\Omega)^3 \) with \( p > 2 \), such that \( \tilde{z}^i \in H^1(\Omega)^3 \) and
\begin{equation}
\int_{\Omega} \frac{4}{\Delta t^2} \tilde{\eta} \, dx + \int_{\Omega} \nabla \tilde{z}^n \nabla \tilde{\eta} \, dx + \int_{\Omega} \frac{1}{2\varepsilon} (\tilde{u}^n + \tilde{u}^{n+1})^2 +
\frac{1}{2} (\tilde{u}^n + \tilde{u}^{n-1})^2 - 2) \tilde{z}^n \tilde{\eta} \, dx = \int_{\Omega} \frac{4}{\Delta t^2} \tilde{u}^n \tilde{\eta}, \quad \forall \tilde{\eta} \in H_0^1(\Omega)^3.
\end{equation}

Under the assumptions \(\tilde{u}^n, \tilde{u}^{n-1} \in L_p(\Omega)^3\), and for \(\tilde{z}^n, \tilde{\eta} \in H^1(\Omega)^3\), the integral
\begin{equation}
\int_{\Omega} \left(\frac{1}{2} (\tilde{u}^n + \tilde{u}^{n+1})^2 + \frac{1}{2} (\tilde{u}^n + \tilde{u}^{n-1})^2\right) \tilde{z}^n \tilde{\eta} \, dx
\end{equation}
is well-defined, because of the Hölder inequality (\(\int uvw \leq ||u||_{L_p} ||v||_{L_p} ||w||_{L_p}\),\(1/p_1 + 1/p_2 + 1/p_3 = 1\)) and continuous embedding \(H^1(\Omega) \subset L_q(\Omega)\) for any \(q < \infty\).

From (3.2) we have that \(\tilde{u}^1 = \tilde{u}_0 + \Delta \tilde{u}_1 + 1/2\Delta^2 \tilde{u}_0;\) if \(\tilde{u}_1 \in L_p(\Omega)^3\) and \(\Delta \tilde{u}_0 \in L_p(\Omega)^3\), then \(\tilde{u}^0, \tilde{u}^1 \in L_p(\Omega)^3\).

Furthermore, we suppose that \(||\Delta \tilde{u}_0 - \Delta \tilde{u}_0||_{L_p} \to 0\) and \(||\tilde{u}_1 - \tilde{u}_1||_{L_p} \to 0\) as \(h \to 0\). This ensures the uniform boundness in \(h\) in the \(L_p\)-norm of the sequences \(\{\tilde{u}_1\}_h\) and \(\{\Delta \tilde{u}_0\}_h\).

Now, choosing \(\tilde{v}_h = \tilde{z}^n_h\) for (3.5) we obtain
\begin{equation}
\frac{4}{\Delta t^2} - \frac{1}{\varepsilon} S_h(||\tilde{z}^n||^2) + ||\nabla \tilde{z}^n_h||_{L_2}^2 \leq \frac{4}{\Delta t^2} S_h(||\tilde{u}^n||_{L_2}||\tilde{z}^n||_{L_2}).
\end{equation}

Under the induction assumption \(||\tilde{u}^n_h||_{L_p} \leq c \neq c(h)\) (using the inequality \(\Delta t \leq 2\sqrt{\varepsilon}\)) we get the uniform in \(h\) estimate
\begin{equation}
||\nabla \tilde{z}^n_h||_{L_2} \leq c \neq c(h).
\end{equation}

Using this estimate and the induction assumptions \(||\tilde{u}^{n-1}_h||_{L_p}, ||\tilde{u}^n||_{L_p} \leq c \neq c(h)\) we can choose from the sequence \(\{\tilde{u}^{n+1}_h\}_h\) a subsequence (we keep the same notation for it) such that
\begin{equation}
\tilde{z}^{n+1}_h \to \tilde{z}^{n+1} = 1/4(\tilde{u}^{n+1} + 2\tilde{u}^n + \tilde{u}^{n-1}) \quad \text{weakly in } H^1(\Omega)^3
\end{equation}
\begin{equation}
\tilde{u}^{n+1}_h \to \tilde{u}^{n+1} \quad \text{strongly in } L_p(\Omega)^3.
\end{equation}

Now, passing to the limit as \(h \to 0\) in equation (3.5) with \(\tilde{v}_h \to \tilde{v}\) strongly in \(H^1(\Omega)^3\), we derive the weak form of equation (3.1).

3) Under the assumptions of this section we prove that the sequences \(\{||\tilde{u}^0||_{L_2}\}_h\) and \(\{||\tilde{u}^1||_{L_2}\}_h\) are uniformly bounded in \(h\). So, \(E^{1/2}_h \leq c \neq c(h)\) and as a consequence of (3.8) \(E^{n+1/2}_h \leq c \neq c(h,n)\) for any \(n\). This means that \(||\tilde{u}^n_h||_{L_2} \leq c \neq c(h,n)\) and we can choose the subsequences of \(\{\tilde{u}^n_h\}_h\), which converge weakly in \(H^1(\Omega)^3\) for any \(n\). The rest of the proof is the same as in the previous case.
Remark 3.2. When $\bar{u}_1 \in H^1(\Omega)^3$ and $\Delta u_0 \in H^1(\Omega)^3$ the energy $E^n$ in (3.3) is well defined and the energy preserving property (3.4) holds for any $n$. Direct calculations show that

$$E^{1/2} = \frac{1}{2} \int_{\Omega} \left| \frac{\bar{u}^{n+1} - \bar{u}^n}{\Delta t} \right|^2 \, dx + \frac{1}{2} \int_{\Omega} \left| \nabla \frac{\bar{u}^{n+1} + \bar{u}^n}{2} \right|^2 \, dx + \frac{1}{\epsilon} c_1 \Delta t^4 =$$

$$\int_{\Omega} |\bar{u}^{n+1}|^2 \, dx + \int_{\Omega} |\nabla \bar{u}^n|^2 + \frac{1}{\epsilon} (c_2 \Delta t^4 + c_3 \Delta t) \tag{3.12}$$

with constants $c_1, c_2$ and $c_3$ depending on $H^1(\Omega)^3$-norms of $\bar{u}_1$ and $\Delta u_0$. As a consequence of (3.4) and (3.12) we have the following estimate

$$\int_{\Omega} \left( \left| \frac{\bar{u}^{n+1} + \bar{u}^n}{2} \right|^2 - 1 \right)^2 \, dx \leq 2\epsilon \left( \int_{\Omega} \left| \frac{\bar{u}^{n+1} - \bar{u}^n}{\Delta t} \right|^2 \, dx + \int_{\Omega} \left| \nabla \frac{\bar{u}^{n+1} + \bar{u}^n}{2} \right|^2 \, dx \right) + O(\Delta t^4)$$

$$= 2\epsilon \left( \int_{\Omega} |\bar{u}^{n+1}|^2 \, dx + \int_{\Omega} |\nabla \bar{u}^n|^2 \right) + O(\Delta t) \text{ for all } n \geq 2 \tag{3.13}$$

Remark 3.3. The energy preserving properties (3.4) and (3.8) ensure the unconditional stability of schemes (3.1) and (3.5) respectively.

It follows from the proof of Proposition 3.1 that a solution of the semidiscrete problem (3.1) is a weak limit when $h \to 0$ of solutions of the fully discrete problem (3.5).

When assumptions $\bar{u}_1 \in H^1(\Omega)^3$ and $\Delta u_0 \in H^1(\Omega)^3$ hold, we get from (3.4) the uniform boundness in $\Delta t$ (or, equivalently, in $n$) of the sequences $\{||\frac{\bar{u}^{n+1} - \bar{u}^n}{\Delta t}||_0\}$ and $\{||\nabla \frac{\bar{u}^{n+1} + \bar{u}^n}{2}||_0\}$. Using this result, we can prove that a solution of problem (2.2) – (2.5) is a weak limit (for the corresponding norms) of a subsequence of solutions to problem (3.1).

Proposition 3.2. Let $\bar{u}^1 \in H^1(\Omega)^3$ and $\Delta \bar{u}_0 \in H^1(\Omega)^3$. There exists a constant $\tilde{c}$, independent of $\Delta t$ and $\epsilon$, such that for $\Delta t \leq \tilde{c} \epsilon$ problems (3.1) and (3.5) have unique solutions.

Proof. We prove the uniqueness result only for problem (3.1), the proof for (3.5) being similar.

Let $\bar{u}_1^{n+1}$ and $\bar{u}_2^{n+1}$ be two solutions of (3.1), and $\bar{w} = \bar{u}_1^{n+1} - \bar{u}_2^{n+1}$; assume that $\bar{u}_1^k = \bar{u}_2^k$ for all $k \leq n$. From (3.1) we obtain

$$\frac{1}{\Delta t^2} ||\bar{w}||_0^2 + ||\nabla \bar{w}||_0^2 \leq \frac{1}{\epsilon} ||\bar{w}||_0^2 +$$
\[
\frac{c}{\varepsilon} \int_{\Omega} |\tilde{w}|^2 \left( \tilde{u}''_{1} + \tilde{u}''_{2} + 2\tilde{u}'_{1} \right) + 2\tilde{u}'_{2} + 2\tilde{u}''_{2} \, dx
\]  \hspace{1cm} \text{(3.14)}

We estimate the right-hand side of (3.14) (denoted by \( S \)) by using the Hölder inequality, the continuous embedding \( H^1(\Omega) \subset L^q(\Omega), \forall q < +\infty \), and the uniform boundness in \( n \) of the \( H^1(\Omega)^3 \)-norms for the solutions of (3.1):

\[
S \leq \frac{1}{\varepsilon} ||\tilde{w}||_0^2 + \frac{c}{\varepsilon} \max \left( ||\tilde{u}'_{1}||_1^2 + ||\tilde{u}'_{2}||_1^2 \right) ||\tilde{w}||_1 \leq \frac{c}{\varepsilon} ||\tilde{w}||_0^2 + ||\tilde{w}||^2_1.
\]

Here \( c \) is a generic constant, not dependent on \( n \) and \( \varepsilon \). Now it is easy to see that for \( \Delta t \leq \bar{\varepsilon} \varepsilon \), we have \( ||\tilde{w}||_0 \leq 0 \) with appropriate \( \bar{\varepsilon} \). \( \Box \)

4. SOLUTION METHOD FOR THE FULLY DISCRETE PROBLEM

We solve equation (3.5) for \( n \geq 1 \). Hereafter we drop the index \( h \) from the functions. Let us introduce at each time step the auxiliary variable \( \bar{z} = (\tilde{u}''_{1} + 2\tilde{u}'_{2} + \tilde{u}'_{2})/4 \), then problem (3.5) can be written as follows

\[
(4\bar{z} - 4\tilde{u}'') - \Delta^2 \Delta_h \bar{z} + \frac{\Delta^2}{2\varepsilon} \left( |2\bar{z} - \tilde{u}'_{2}|^2 + |\tilde{u}'_{2}|^2 - 2 \right) \bar{z} = 0,
\]  \hspace{1cm} \text{(4.1)}

where \( \tilde{u}'_{2} = (\tilde{u}'_{2} + \tilde{u}'_{2})/2 \), and \( -\Delta_h \) is the discrete Laplace operator. Equation (4.1) is completed by Dirichlet boundary conditions. Let us now denote the left-hand side of (4.1) by \( F(\bar{z}) \). Obviously, function \( F(\bar{z}) \) is differentiable and

\[
F'(\bar{z}) \bar{w} = 4\bar{w} - \Delta^2 \Delta_h \bar{w} + \frac{\Delta^2}{2\varepsilon} \left( |2\bar{z} - \tilde{u}'_{2}|^2 + |\tilde{u}'_{2}|^2 - 2 \right) \bar{w} + \frac{2}{\varepsilon} \Delta^2 (2\bar{z} - \tilde{u}'_{2}, \bar{w}) \bar{z},
\]

where \( (\cdot, \cdot) \) is the inner product in \( R^3 \) and matrix \( F'(\bar{z}) \) has the form

\[
(4 + \frac{\Delta^2}{2\varepsilon} \left( |2\bar{z} - \tilde{u}'_{2}|^2 + |\tilde{u}'_{2}|^2 - 2 \right)) I - \Delta^2 \Delta_h
\]  \hspace{1cm} \text{(4.2)}

\[
+ \frac{4\Delta^2}{\varepsilon} \bar{z}^T \bar{z} - \frac{2}{\varepsilon} \Delta^2 \bar{z}(\tilde{u}'_{2})^T,
\]

with the unit matrix \( I \). Under assumption \( \Delta t \leq 2\sqrt{\varepsilon} \) matrix \( F'(\bar{z}) \) is positive definite but not symmetric due to the term \( (2/\varepsilon)\Delta^2 \bar{z}(\tilde{u}'_{2})^T \). In order to solve equation \( F(\bar{z}) = 0 \) we use the following quasi-Newton method

\[
F'_0(\bar{z}^k)(\bar{z}^{k+1} - \bar{z}^k) + F(\bar{z}^k) = 0, \quad k = 0, 1, 2, \ldots
\]  \hspace{1cm} \text{(4.3)}
where

\[ F_0'(\tilde{z}) = \frac{4}{\varepsilon} \left( \frac{\Delta t^2}{2} \left( 2\tilde{z} - \bar{u}^{n-1/2} \right)^2 + |\bar{u}^{n-1/2}|^2 - 2 \right) I - \Delta t^2 \Delta_h + \frac{2\Delta t^2}{\varepsilon} \tilde{z}^T, \]

which is obviously positive definite for \( \Delta t \leq 2\sqrt{\varepsilon} \). Clearly, \( F_0'(\tilde{z}) \) differs from \( F'(\tilde{z}) \) by the term \( \frac{1}{\varepsilon} \Delta t^3 \left( \frac{\bar{u}^{n+1} + 2\bar{u}^n + \bar{u}^{n-1}}{4} \right) \left( \frac{\tilde{z} - \bar{u}^{n-1/2}}{2\Delta t} \right)^T \) at the exact solution and is expected to be "small" enough when starting from a "good" initial guess. To solve problem (4.3) at each time step we use a conjugate gradient algorithm.

5. NUMERICAL RESULTS

We have performed numerical experiments for problem (2.2)-(2.5) in \( \Omega = (0,1) \times (0,1) \) by using finite difference in space for (3.1) with a uniform mesh step size \( h \). This difference scheme can be treated as a finite element scheme with \( P_1 \)-interpolation and trapezoidal quadrature formulae to approximate the integrals. We considered different input data and different mesh and time step sizes \( h \) and \( \Delta t \), and penalty parameter \( \varepsilon > 0 \). We have found that our numerical results agree very well with the constrained verification estimate (3.13). Moreover, our calculations showed that the discrete scheme is stable and that the iterative method (4.3) is convergent with a high rate of convergence under much less restrictive conditions between \( h \), \( \Delta t \), and \( \varepsilon \) than those given by developed theory. Figures 1-7 show the energy and \( \max_x |\bar{u}|^2 - 1 \) behavior in time, the shape of \( u_3 \) component of \( \bar{u} \) for different values of \( \varepsilon \) with the initial data defined as follows

\[ u_1^0 = \frac{x-x^*}{r}, \quad u_2^0 = \frac{y-y^*}{r}, \quad u_3^0 = \frac{\cos(\pi x - \pi y)}{r}, \quad \bar{u}_1 = 0, \]

and boundary data given by:

\[ g_1 = \frac{x-x^*}{r}, \quad g_2 = \frac{y-y^*}{r}, \quad g_3 = \frac{\cos(\pi x - \pi y)}{r}, \]

with \( r = \sqrt{(x-x^*)^2 + (y-y^*)^2 + \cos^2(\pi x - \pi y)} \) and \((x^*,y^*) = (1,1,1)\).

**Remark 5.1.** On both Figures 1 (which show the history of the discrete energy and deviation from the constraint \( |\bar{u}|^2 = 1 \)), we observe oscillations taking place at the beginning of the evolution. These oscillations damped out as \( t \) increases. In order to reduce this unwanted phenomenon we have modified scheme (3.1), (3.2) as follows:
We started (3.1) from $n = 0$, instead of $n = 1$.

- We used $\bar{u}^0 = \bar{u}_0$ and $\bar{u}^1 - \bar{u}^{-1} = 2\Delta t \bar{u}_1$ as initial conditions.

This modification slightly improves the numerical result (level of oscillations at the start is reduced by about 10%).

**Acknowledgments.** The authors would like to thank Professor Jalal Shatah for suggesting us to look to problems such as (2.1)-(2.3); the support of LACSI/DOE (Contract No. 74837-001-0349 from the Regents of University of California) and Allied Geophysical Laboratory at University of Houston is also acknowledged, as are the helpful comments and suggestions from Professors Mikhael Balabane and Patrick Joly.
A penalty approach

Figure 3. Energy behavior (left) and $\max_x |\tilde{u}_j^2 - 1|$ (right) for $\varepsilon = 10^{-5}$, $h = 1/50$, $\Delta t = 1/100$

Figure 4. $u_3$ component of $\tilde{u}$ at $t = 1/4$ (left) and $t = 1/2$ (right) for $\varepsilon = 10^{-3}$, $h = 1/50$, $\Delta t = 1/100$

REFERENCES

Figure 5. $u_3$ component of $\vec{u}$ at $t = 3/4$ (left) and $t = 1$ (right) for $\varepsilon = 10^{-3}$, $h = 1/50$, $\Delta t = 1/100$

Figure 6. $u_3$ component of $\vec{u}$ at $t = 1/4$ (left) and $t = 1/2$ (right) for $\varepsilon = 10^{-5}$, $h = 1/50$, $\Delta t = 1/100$

Figure 7. $u_3$ component of $\vec{u}$ at $t = 3/4$ (left) and $t = 1$ (right) for $\varepsilon = 10^{-5}$, $h = 1/50$, $\Delta t = 1/100$