

## Application of Sobolev Gradient Method to Solve Klein Gordon Equation

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**Abstract.** To find the minima of an energy functional, is a well known problem in physics and engineering. Sobolev gradients have proven to be affective to find the critical points of a functional. Here, we introduce a similar approach to find the solution of nonlinear Klein Gordon equation (NKGE) in a finite-element setting. The results are compared using Euclidean, weighted and unweighted Sobolev gradients. We also compare the results with Newton's method for a test problem and show that the presented method is better than Newton's method in this case.

**AMS (MOS) Subject Classification Codes:** 4601; 65M06

**Key Words:** Sobolev gradient; Nonlinear Klein Gordon Equation; Finite-element setting; Steepest descent.

### 1. INTRODUCTION

In recent years, the most of the universe problems can be described by nonlinear evolution equations. These equations play a vital role in different fields, such as solid state physics, plasma physics, fluid mechanics, optical fibers, geochemistry and chemical kinetics. These problems are difficult to solve both analytically and numerically. Recently, various numerical algorithms have been developed for approximation of solutions of nonlinear problems. One of the example is the Sobolev gradient method. Sobolev gradients have been utilized to solve linear and nonlinear singular differential equations [12]. In some cases, better results can be obtained by choosing appropriate weights in the construction of the Sobolev space in which steepest descent occurs. Newton's method fails to converge in few cases for which the Sobolev gradient method converges. The Sobolev gradient approach has been successfully used for the solution of NKGE in a Finite-difference setting [18]. The purpose of this paper is to give a related approach in a finite-element setting for higher dimensional NKGE.

Sobolev gradient methods [15] have been used in finite-difference [12] and finite-element settings [2] for the solution of partial differential equations (PDEs). Successful applications of the Sobolev gradient method can be seen in materials science [24, 25, 19, 26, 3], physics [8, 9, 10, 5, 14, 13], geometric modelling [22], image processing [20, 21] and Differential Algebraic Equations (DAEs)[16]. A detailed discussion of Sobolev gradient

methods can be found in [15]. This reference contains existence and sufficient conditions for convergence of the solution. The reader can refer to [23] for further applications and open problems in this field.

Computational work was done on an Intel(R) 3 GHz Core(TM)2 Duo machine with 1 GB RAM. We used the open sources FreeFem++ [7] software for the solution of PDEs. All the graphs are drawn using gnuplot software.

## 2. SOBOLEV GRADIENT APPROACH

The concept of Sobolev gradient and steepest descent is discussed in this section. A detailed description of Sobolev gradients can be found in [15]. The gradient  $\nabla\mathcal{F}$  of a real valued  $C^1$  function  $\mathcal{F}$  on  $R^n$  where  $n$  is a positive integer, is given by

$$\lim_{t \rightarrow 0} \frac{1}{t} (\mathcal{F}(x + th) - \mathcal{F}(x)) = \mathcal{F}'(x)h = \langle h, \nabla\mathcal{F}(x) \rangle_{R^n}, \quad x, h \in R^n. \quad (2.1)$$

Let  $\langle \cdot, \cdot \rangle_S$  be an inner product on  $R^n$  different from the standard inner product  $\langle \cdot, \cdot \rangle_{R^n}$ . Then there is a function  $\nabla_S\mathcal{F} : R^n \rightarrow R^n$  such that

$$\mathcal{F}'(x)h = \langle h, \nabla_S\mathcal{F}(x) \rangle_S \quad x, h \in R^n. \quad (2.2)$$

The linear functional  $\mathcal{F}'(x)$  can be represented using any inner product on  $R^n$ . Let  $\nabla_S\mathcal{F}$  be the gradient of  $\mathcal{F}$  with respect to the inner product  $\langle \cdot, \cdot \rangle_S$ . Considering the linear transformation  $A : R^n \rightarrow R^n$ , these two inner products can be related as follows:

$$\langle x, y \rangle_S = \langle x, Ay \rangle_{R^n}$$

for  $x, y \in R^n$  and a reflection leads to

$$(\nabla_S\mathcal{F})(x) = A^{-1}\nabla\mathcal{F}(x), \quad x \in R^n. \quad (2.3)$$

For every  $x \in R^n$ , there is an inner product  $\langle \cdot, \cdot \rangle_x$  on  $R^n$ . For  $x \in R^n$ , we define  $\nabla_x\mathcal{F} : R^n \rightarrow R^n$  as follows:

$$\mathcal{F}'(x)h = \langle h, \nabla_x\mathcal{F}(x) \rangle_x \quad \text{for } x, h \in R^n. \quad (2.4)$$

There is a variety of gradients for  $\mathcal{F}$  depending upon the choice of metric and these gradients have quite different numerical properties. Such a gradient of a functional which is defined in a finite or an infinite dimensional Sobolev space, is called a Sobolev gradient. Sobolev spaces are discussed in detail in [1]. Steepest descent can be categorized into two types: discrete steepest descent and continuous steepest descent.

Let  $\nabla_S\mathcal{F}$  be the gradient of a real-valued  $C^1$  function  $\mathcal{F}$  on a Hilbert space  $H$  with respect to the inner product  $\langle \cdot, \cdot \rangle_S$  defined on  $H$ . Discrete steepest descent can be regarded as a process of constructing a sequence  $\{x_k\}$  such that  $x_0$  is given and

$$x_k = x_{k-1} - \delta_k(\nabla\mathcal{F})(x_{k-1}), \quad k = 1, 2, \dots \quad (2.5)$$

where  $\delta_k$  is chosen for each  $k$  so that it minimizes, if possible,

$$\mathcal{F}(x_{k-1} - \delta_k(\nabla\mathcal{F})(x_{k-1})). \quad (2.6)$$

Continuous steepest descent is a process of constructing a function  $z : [0, \infty) \rightarrow H$  such that

$$\frac{dz}{dt} = -\nabla \mathcal{F}(z(t)), \quad z(0) = z_{initial}. \quad (2.7)$$

$z(t) \rightarrow z_\infty$  under suitable conditions on  $F$ , where  $F(z_\infty)$  is the minimum value of  $F$ . The limiting case of discrete steepest descent can be treated as continuous steepest descent and, therefore, we can consider (2.5) as a numerical scheme for approximating solutions to (2.7). Continuous steepest descent gives a theoretical starting point to prove the convergence of discrete steepest descent.

According to (2.5), we find  $u = \lim_{k \rightarrow \infty} x_k$  such that

$$\mathcal{F}(u) = 0 \text{ or } (\nabla_S \mathcal{F})(u) = 0 \quad (2.8)$$

and for (2.7), we find  $u = \lim_{t \rightarrow \infty} z_t$  such that (2.8) holds.

We construct  $\mathcal{F}$  by a variational principle to solve a partial differential equation (PDE), and we have a function  $u$  that satisfies the differential equation if and only if  $u$  is a critical point of  $\mathcal{F}$ . In these situations, we use steepest descent minimization process to find a zero of the gradient of  $\mathcal{F}$ . In our case

$$\begin{aligned} \mathcal{F}(u) = \int_{\Omega} \delta_t^2 \gamma \frac{u^{k+1}}{k+1} + (1 + \beta \delta_t^2) \frac{u^2}{2} - 2f_1 u + f_2 u \\ - \delta_t^2 h(x, t) u - \delta_t^2 \frac{\alpha}{2} |\nabla u|^2 \end{aligned} \quad (2.9)$$

Note that other functionals are also possible and one of the prime example in this direction is the least square formulation. Such functions are given in [19, 13]. In this paper, we only show results from which  $\mathcal{F}$  comes by a variational principle as the result in this setting are optimal [19]. The existence and convergence of  $z(t) \rightarrow z(\infty)$  for different linear and nonlinear forms of  $\mathcal{F}$  is discussed in [15].

We used only discrete Sobolev spaces in this paper and finite dimensional versions of functionals  $\mathcal{F}$  are considered for numerical computation.

### 3. THE NONLINEAR KLEIN-GORDON EQUATION

Consider the problem

$$\frac{\partial^2 u}{\partial t^2} + \alpha \nabla^2 u + \beta u + \gamma u^k = f(x, t), \quad x \in \Omega = [a, b], \quad 0 < t \leq T \quad (3.10)$$

with initial conditions

$$\begin{cases} u(x, y, 0) = h_1(x), & x \in \Omega \\ u_t(x, y, 0) = h_2(x), & x \in \Omega, \end{cases}$$

and Dirichlet boundary conditions

$$u(x, y, t) = g(x, y, t), \quad x \in \partial\Omega, \quad 0 < t \leq T,$$

where  $\alpha, \beta, \gamma$  and  $\delta_t$  are real constants, and  $f, h_1, h_2, g$  are known functions while  $u$  is unknown. Also we have quadratic nonlinearity for  $k = 2$  and cubic nonlinearity for

$k = 3$ .

This equation describes the motion of scalar spinless particles. It has some useful applications in plasma physics, combined with Zakharov equation representing the interaction of the ion acoustic wave and Langmuir wave in a plasma [17], in astrophysics interacting with Maxwell equation describing a minimally coupled charged boson field to a spherically symmetric space time [4]. Mathematician did a series study for the solution of NKGE. J. Ginibre et al. [6] studied the Cauchy problem for a class of NKGE by a contraction method and find the existence and uniqueness of strongly continuous global solutions. Different numerical algorithms were developed for the solution of NKGE in last 50 years. Strauss et al. [27] proposed a finite difference scheme for the one dimensional NKGE. Numerical treatment for damped NKGE, based on finite element approach is studied in [11, 28].

The aim of the present paper is to extend the Sobolev gradient method to find the solution of NKGE. The method is very simple to apply and can be extended to other kind of nonlinear evolution equations from mathematical physics. An associated functional is formed on  $\Omega$  subject to Dirichlet type of boundary conditions. The functional is given by (2.9). In this equation  $u$  is the desired solution at time  $t + \delta_t$  and  $f_1, f_2$  are solutions at time  $t$  and  $t - \delta_t$ . From now to onwards we denote the functional defined by (2.9) with  $G(u)$ .

**3.1. Gradients and minimization.** In steepest descent, the process of minimization speeds up if we choose a suitable Sobolev space in which the gradient is defined. Mahavier introduced the concept of weighted Sobolev gradients. Following his idea, we define a new inner product suitable for the functional (2.9). A Sobolev space  $H^1(\Omega)$  is defined as follows:

$$H^1(\Omega) = \{u \in L^2(\Omega) : D^\alpha u \in L^2(\Omega), 0 \leq \alpha \leq 1\} \quad (3.11)$$

where  $L^2$  is the Euclidean space (the vector space  $R^M$  equipped with inner product  $\langle u, v \rangle = \sum_i u(i)v(i)$ ). Also  $D^\alpha$  is the weak derivative of  $u$  of order  $\alpha$  and  $H^1(\Omega)$  is a Hilbert space with norm defined by

$$\|u\|_{H^1}^2 = \int_{\Omega} |\nabla u|^2 + |u|^2. \quad (3.12)$$

Keeping in mind Mahavier's idea of weighted gradients, we define a norm which takes care of  $w = \alpha \delta_t$  that is affecting the derivative term in (2.9). Define a weighted Sobolev space  $H^{1,w}(\Omega)$  whose norm is

$$\|u\|_{H^{1,w}}^2 = \int_{\Omega} |w \nabla u|^2 + |u|^2. \quad (3.13)$$

It can be easily verified, that the weighted Sobolev space with the norm defined by (3.13) is a Hilbert space. Now we define a perturbation subspace  $L_0^2(\Omega)$  of functions in order to incorporate the Dirichlet boundary conditions as follows:

$$L_0^2(\Omega) = \{v \in L^2(\Omega) : v = 0 \text{ on } \Gamma\}, \quad (3.14)$$

where  $\Gamma$  denotes the boundary of the domain  $\Omega$ . Perturbation subspaces related to  $H^1$  and  $H^{1,w}$  are  $H_0^1 = L_0^2 \cap H^1$  and  $H_0^{1,w} = L_0^2 \cap H^{1,w}$  respectively.

The idea is to find a function  $u$  that minimizes the energy functional (2.9), the gradient  $\nabla G(u)$  of a functional  $G(u)$  associated with the original problem and to find the zero of the gradient. We need to define the Fréchet derivative for this purpose. The Fréchet derivative of  $G(u)$  is a bounded linear functional  $G'(u)$  defined as follows:

$$G'(u)h = \lim_{\theta \rightarrow 0} \frac{G(u + \theta h) - G(u)}{\theta} \text{ for } h \in H_0^1(\Omega). \quad (3.15)$$

Using (3.15), we get

$$\begin{aligned} G'(u)h &= \lim_{\theta \rightarrow 0} \int_{\Omega} \delta_t^2 \gamma \frac{(u + \theta h)^{k+1}}{k+1} + (1 + \beta \delta_t^2) \frac{(u + \theta h)^2}{2} \\ &\quad - 2f_1(u + \theta h) + f_2(u + \theta h) - \delta_t^2 h(x, t)(u + \theta h) \\ &\quad - \delta_t^2 \frac{\alpha}{2} |\nabla(u + \theta h)|^2 - \delta_t^2 \gamma \frac{u^{k+1}}{k+1} - (1 + \beta \delta_t^2) \frac{u^2}{2} \\ &\quad + 2f_1 u - f_2 u + \delta_t^2 h(x, t)u + \delta_t^2 \frac{\alpha}{2} |\nabla u|^2. \end{aligned} \quad (3.16)$$

Simplifying the above expression gives

$$\begin{aligned} G'(u)h &= \int_{\Omega} \delta_t^2 \gamma u^k + (1 + \beta \delta_t^2)u - 2f_1 + f_2 - \delta_t^2 h(x, t) \\ &\quad + \int_{\Omega} \alpha \delta_t^2 \nabla u \cdot \nabla h. \end{aligned} \quad (3.17)$$

Let  $\nabla G(u)$ ,  $\nabla G_s(u)$  and  $\nabla G_w(u)$  denote the gradients in  $L^2$ ,  $H^1$  and  $H^{1,w}$  respectively. Then by using (2) we can write

$$\dot{G}(u)h = \langle \nabla G(u), h \rangle_{L^2} = \langle \nabla G_s(u), h \rangle_{H^1} = \langle \nabla G_w(u), h \rangle_{H^{1,w}}. \quad (3.18)$$

Thus the gradient in  $L^2$  is

$$\nabla G(u) = \delta_t^2 \gamma u^k + (1 + \beta \delta_t^2)u - 2f_1 + f_2 - \delta_t^2 h(x, t) - \alpha \delta_t^2 \nabla^2 u.$$

As Dirichlet boundary conditions are being used in our problem. At the boundaries of the system,  $u$  has fixed values and we desire gradients that zero at the boundary of  $\Omega$ . Thus we shall not use  $\nabla G(u)$ . Instead  $\pi \nabla G(u)$  will be used where  $\pi$  is a projection which sets boundary points zero. We use Freefem++[7] which is a freely available software particularly designed for the solution of partial differential equations using the finite element method. The software facilitates setting the gradient to zero at the boundary. Therefore, in order to find  $\pi \nabla G(u)$ , we solve

$$\begin{aligned} \pi \left( \int_{\Omega} \delta_t^2 \gamma u^k + (1 + \beta \delta_t^2)u - 2f_1 + f_2 - \delta_t^2 h(x, t) + \int_{\Omega} \alpha \delta_t^2 \nabla u \cdot \nabla h \right) = \\ \pi \int_{\Omega} \nabla G(u)h + \int_{\Omega} \nabla \nabla G(u) \cdot \nabla h. \end{aligned} \quad (3.19)$$

For  $u$  in  $L^2(\Omega)$ , we find  $\nabla G(u) \in L_0^2$  such that

$$\langle \nabla G(u), h \rangle_{L^2} = \langle A(u) - f, h \rangle_{L^2}, \quad \forall h \in L_0^2(\Omega) \quad (3.20)$$

$$\begin{aligned} \langle A(u), h \rangle_{L^2} = & \int_{\Omega} \delta_t^2 \gamma u^k + (1 + \beta \delta_t^2) u - 2f_1 + f_2 \\ & - \delta_t^2 h(x, t) + \int_{\Omega} \alpha \delta_t^2 \nabla u \cdot \nabla h. \end{aligned} \quad (3.21)$$

Steepest descent using this gradient is inefficient, as the CFL condition applies. We need to find gradients in  $H^1$  and  $H^{1,w}$ . By using (3.12) and (3.18) we can relate the  $L^2$  gradient and unweighted Sobolev gradient in the weak form as

$$\langle (1 - \nabla^2) \nabla_s G(u), h \rangle_{L^2} = \langle A(u) - f, h \rangle_{L^2}. \quad (3.22)$$

similarly using (3.13) and (3.18) one can relate the weighted Sobolev gradient with the  $L^2$  gradient

$$\langle (1 - w^2 \nabla^2) \nabla_w G(u), h \rangle_{L^2} = \langle A(u) - f, h \rangle_{L^2}. \quad (3.23)$$

For numerical implementation of the method, we find gradients in unweighted and weighted Sobolev spaces. In order to find gradients we need to solve the following equations.

$$\begin{aligned} \pi \left( \int_{\Omega} \delta_t^2 \gamma u^k + (1 + \beta \delta_t^2) u - 2f_1 + f_2 - \delta_t^2 h(x, t) + \int_{\Omega} \alpha \delta_t^2 \nabla u \cdot \nabla h \right) = \\ \pi \int_{\Omega} \nabla_s G(u) h + \int_{\Omega} \nabla_s \nabla G(u) \cdot \nabla h. \end{aligned} \quad (3.24)$$

$$\begin{aligned} \pi \left( \int_{\Omega} \delta_t^2 \gamma u^k + (1 + \beta \delta_t^2) u - 2f_1 + f_2 - \delta_t^2 h(x, t) + \int_{\Omega} \alpha \delta_t^2 \nabla u \cdot \nabla h \right) = \\ \pi \int_{\Omega} \nabla_w G(u) h + \int_{\Omega} \nabla_w \nabla G(u) \cdot \nabla h. \end{aligned} \quad (3.25)$$

So the algorithm is as follow

- Find  $\nabla_s G(u)$  or  $\nabla_w G(u)$  by solving (3.24) or (3.25)
- Update  $u$  by  $u - \lambda \nabla_s G(u)$  or  $u - \lambda \nabla_w G(u)$ , where  $\lambda$  is step size towards minimum
- Repeat till convergence.

Note that, in case of weighted Sobolev gradients, by increasing resolution of the system one does not need to reduce the value of  $\lambda$  therefore the number of minimization steps to reach convergence remains reasonable.

#### 4. NUMERICAL RESULTS

In first case, we let  $\Omega$  be a square centered at the origin of each side length 10. The initial condition was  $u = \sin x \cos 2y$  and the Dirichlet condition was that  $u = -1$  and  $u = 1$  on opposite sides. We let  $\alpha = 0.1$ ,  $\beta = \gamma = 1$  and  $f(x, t) = 0$ . The system evolved over three time steps with  $\delta_t = 0.5$ . For each time step  $\delta_t$  the functional defined by (2.9) for cubic nonlinearity ( $k = 3$ ) was minimized using gradients in  $L^2$ ,  $H^1$  and  $H^{1,w}$  space until the infinity norm of the gradient vector became less than some fixed number.

For solving problem numerically using FreeFem++, a grid is formed by specifying the number of nodes on each border. FreeFem++ then creates a mesh and solves the system such as (3.25) which determine the  $H^1$  and  $H^{1,w}$  gradients. We did numerical experiments with  $M = 8, 16, 32$  and  $64$  nodes on each border. The number of steps taken for convergence by each method, the step-size and the CPU time were recorded in Table (1).

TABLE 1. Numerical results of steepest descent in  $L^2$ ,  $H^1$ ,  $H^{1,w}$  using  $\delta_t=0.5$ ,  $\alpha = 0.1$  for three time steps in the two-dimensional case.

$\lambda$			iterations			CPUs			M	Triangles
$L^2$	$H^1$	$H^{1,w}$	$L^2$	$H^1$	$H^{1,w}$	$L^2$	$H^1$	$H^{1,w}$	-	-
0.066	3.6	0.8	140	52	10	6.0	3.0	0.5	30	1800
0.024	3.6	0.8	387	55	10	39	7.0	1.4	50	5000
0.001	3.6	0.8	932	57	10	172	14	2.6	70	9800
0.0076	3.6	0.8	1228	58	10	351	27	4.1	90	16200

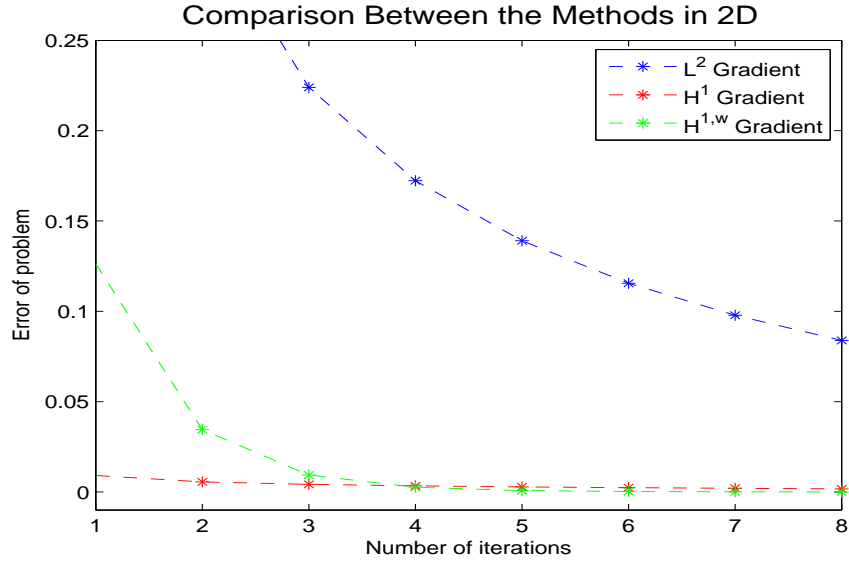


FIGURE 1. Graph of first 8 iterations versus infinity norm of the gradient vector with gradients in  $L^2, H^1, H^{1,w}$ .

From the Table (1), we see that as the mesh becomes finer with increasing  $M$ , more minimization steps are required for convergence of Euclidean gradient. But the best results are using weighted Sobolev gradient. By decreasing the value of  $\alpha$  the weighted gradient becomes more and more efficient over the traditional Sobolev gradient.

Figure (1) shows the results of using steepest descent with the Euclidean, weighted and unweighted Sobolev gradients to solve equation (2.9) in two dimensional case, with an initial iterate of  $u = \sin x \cos 2y$ . It shows the comparison between weighted and unweighted gradients, for first eight iterations versus the infinity norm of the gradient vector. From the graph we see that convergence is slow with the unweighted gradient.

For the three-dimensional case, we let  $\Omega$  be a cube centered at the origin of each side length 10. The initial state was  $u = 1.0$ . We set  $u = 1$  on the top and bottom faces and  $u = -1$  on the left, right, front and back faces of the cube. We let  $\alpha = 0.1$  and time step  $\delta_t = 0.5$ . The system evolved over three time steps. For each time step  $\delta_t$  the functional defined by (2.9) was minimized using gradients in  $H^1$  and  $H^{1,w}$  until the norm of gradient vector becomes smaller than some set positive number. Once again, the finite-element software

TABLE 2. Numerical results of steepest descent in  $L^2$ ,  $H^1$ ,  $H^{1,w}$  using  $\delta_t=0.5$ ,  $\alpha = 0.1$  for three time steps in the three-dimensional case.

$\lambda$			iterations			CPUs			M	Triangles
$L^2$	$H^1$	$H^{1,w}$	$L^2$	$H^1$	$H^{1,w}$	$L^2$	$H^1$	$H^{1,w}$	-	-
0.9	1.9	0.9	18	46	18	0.3	1.36	0.3	5	50
0.7	1.9	0.9	25	93	18	2	10.44	2	10	200
0.4	1.9	0.9	43	112	22	12	38.6	7	15	450
0.2	1.9	0.9	92	130	22	55	106	18	20	800

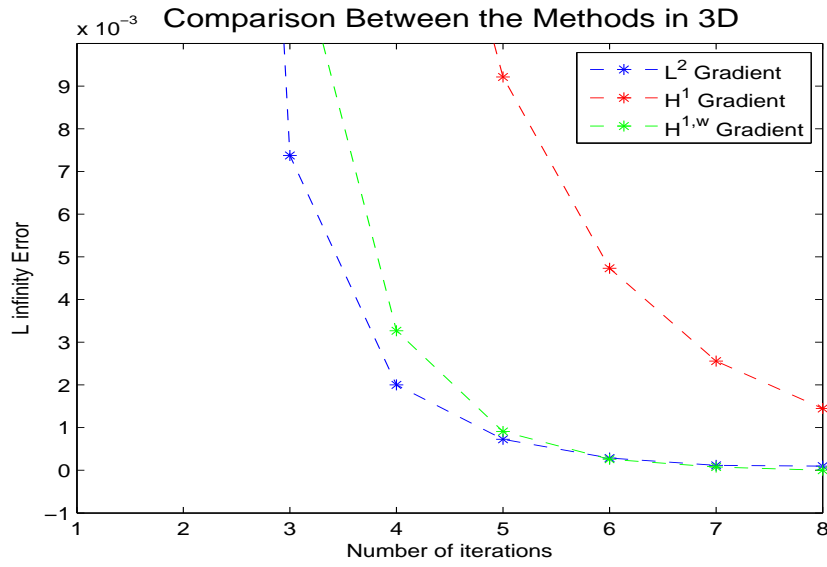


FIGURE 2. Graph of first 8 iterations verses infinity norm of the gradient vector with gradients in  $L^2$ ,  $H^1$ ,  $H^{1,w}$ .

FreeFem++ [7] was used for this problem. We did numerical experiments with  $M = 5, 10, 15$  and  $20$  nodes on each axis. The total number of minimization steps, the largest value of  $\lambda$  that can be used and the CPU time can be seen in Table (2).

Note that as the mesh becomes finer with increasing  $M$ , the weighted Sobolev gradient becomes more and more efficient than the results from  $L^2$  and  $H^1$  gradient. In the case of the weighted Sobolev gradient, the required number of iterations to reach convergence remains reasonable. By reducing the value of  $\alpha$ , the performance of weighted gradient is much better than the other gradients.

In Figure (2) results of using steepest descent for the first eight iterations verses infinity norm of the gradient vector in  $L^2$ ,  $H^1$ ,  $H^{1,w}$  in three dimensional case, with an initial iterate of  $u = 1$  is shown. It is clear from the graph that convergence is fastest with the  $H^{1,w}$  gradient.



TABLE 3. Comparison of Newton's method and steepest descent in  $H^{1,w}$  for different values of  $\alpha$ .

$\alpha = 0.1$		$\alpha = 0.01$		$\alpha = 0.001$		–
Newton	$H^{1,w}$	Newton	$H^{1,w}$	Newton	$H^{1,w}$	Error
31	11	39	10	47	10	$10^{-5}$
31	16	39	17	NC	17	$10^{-8}$
33	24	NC	27	NC	26	$10^{-11}$

## 5. COMPARISON WITH NEWTON'S METHOD

In this section, we show the comparison between the weighted Sobolev gradient method and Newton's method. In many circumstances, Newton's method and its different forms are considered optimal. But the convergence depends on a nice initial guess. In our numerical experiments, we also choose a good initial guess so that we could compare the two methods in a fair manner. Consider the variational form of nonlinear problem as given by

$$\begin{aligned} \langle G(u), h \rangle = & \int_{\Omega} \delta_t^2 \gamma \frac{u^{k+1}}{k+1} h + (1 + \beta \delta_t^2) \frac{u^2}{2} h - 2f_1 u h + f_2 u h \\ & - \delta_t^2 h(x, t) u h - \delta_t^2 \frac{\alpha}{2} |\nabla u|^2 h \end{aligned} \quad (5.26)$$

We need to find the Gateaux derivative such that

$$\langle F'(u_n) c_n, v \rangle = \langle F(u), v \rangle, \quad \forall v \in H_0^1(\Omega). \quad (5.27)$$

We use some appropriate linear solver in order to solve equation (5.27). Thus, Newton's iteration scheme is

$$u_{n+1} = u_n - c_n. \quad (5.28)$$

We work out the example in two dimensional case, for this we let  $\Omega$  be a square centered at the origin of each side length 10. The initial state was  $u = 0.0$ . We set  $u = 0.1$  on the vertical edges and  $u = -0.1$  on the horizontal edges of the square. We let  $\delta_t = 0.5$ . The system was evolved over 2 time steps until the infinity norm of the gradient is less than the set tolerance. Results were obtained on  $30 \times 30$  grid points. Table (3) shows the results for various values of  $\alpha$ . The term NC in the table denotes no convergence.

Results show that the performance of Newton's method is better than the weighted gradient but Newton's method does not converge in case of strict stopping criterion. In terms of minimization steps, the results between two methods are comparable at start but Newton's method fails to damp out low frequency error modes i.e; for strict stopping criterion. Whereas the weighted gradient requires more iterations but it keeps on converging even for very tight stopping criteria. When the value of  $\alpha$  is decreased, the weighted Sobolev gradient manages to converge whereas Newton's method becomes more and more inefficient.

## 6. SUMMARY AND CONCLUSIONS

We have presented minimization schemes in this paper for the energy functional of the NKGE based on the weighted Sobolev gradient method [15]. The descent in  $H^1$  outperforms descent in  $L^2$ , but the best results are by considering the descent in  $H^{1,w}$ . The

performance of Sobolev gradient method compared to the Euclidean gradient becomes better as numerical grid spacing is made finer. In this paper the numerical work provides a systematic way for choosing the underlying space and shows that the appropriate choice of weight functions plays a key role in developing efficient code.

Newton's method converges only when the initial guess is taken sufficiently close to a local minimum. At each step, Newton's method requires evaluation of the inverse of the Hessian matrix, which becomes very expensive sometimes or it may or may not be positive definite. It was shown in [20] that for some problems Newton's method fails to converge near the singularity but the Sobolev gradient method does converge. [19, 13] shows a failure of the Newton's method in case when we increase the number of nodes and have a big jump discontinuity whereas this does not happen in case of the weighted Sobolev gradient method. Therefore, the Sobolev gradient method can be efficiently utilized to solve a big range of problems by using appropriate weight functions.

Satisfactory agreement occurs between the new numerical scheme and other solutions. Moreover, steepest descent converges even for a bad initial guess or for jump discontinuities in the initial guess. This research can be further advanced by the the comparison of the performance of weighted gradient with some nonlinear FAS multigrid method in finite element setting.

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