The Scalar Homotopy Method for Solving Non-Linear Obstacle Problem

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Abstract: In this study, the nonlinear obstacle problems, which are also known as the nonlinear free boundary problems, are analyzed by the scalar homotopy method (SHM) and the finite difference method. The one- and two-dimensional nonlinear obstacle problems, formulated as the nonlinear complementarity problems (NCPs), are discretized by the finite difference method and form a system of nonlinear algebraic equations (NAEs) with the aid of Fischer-Burmeister NCP-function. Additionally, the system of NAEs is solved by the SHM, which is globally convergent and can get rid of calculating the inverse of Jacobian matrix. In SHM, by introducing a scalar homotopy function and a fictitious time, the NAEs are transformed to the ordinary differential equations (ODEs), which can be integrated numerically to obtain the solutions of NAEs. Owing to the characteristic of global convergence in SHM, the restart algorithm is adopted to fasten the convergence of numerical integration for ODEs. Several numerical examples are provided to validate the efficiency and consistency of the proposed scheme. Besides, some factors, which might influence on the accuracy of the numerical results, are examined by a series of numerical experiments.

Keywords: nonlinear obstacle problems, scalar homotopy method, finite difference method, nonlinear algebraic equations, global convergence

1 Introduction

The obstacle problems are known as the nonlinear free boundary problems, and the numerical computations are also known to be difficult and expensive. But, many engineering problems [Zhang (2001)] are mathematically formulated as obstacle problems, such as the filtration dam problem, the subsonic flow problem, the Stefan problem, etc. Therefore, in the past decades, many researchers [Al-Said and

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Noor (2002); Cheng and Xue (2006); Liu (2008a); Xue and Cheng (2004); Zhang (2001)] paid attention on developing numerical schemes for solving the obstacle problems. Zhang (2001) used the multilevel projection method and the finite element method for analyzing two-dimensional obstacle problems, while Al-Said and Noor (2002) used the quartic spline method for solving the fourth order obstacle boundary value problems. Although many successful schemes are proposed, it is still very important to find an efficient and stable numerical method to analyze the obstacle problems. Hence, in this study, we would propose a stable numerical scheme, the combination of the scalar homotopy method (SHM) and the finite difference method (FDM), for efficiently solving the nonlinear obstacle problems.

The nonlinear obstacle problem is mathematically formulated as the nonlinear complementarity problem (NCP) [Ferris and Pang (1997)]. By using the Fischer-Burmeister NCP-function [Fischer (1992)] and FDM, the NCP can be transformed to the nonlinear algebraic equations (NAEs). In confronting with the linear problems, there are plenty algorithms, which can be used to solve the system of linear algebraic equations, since most numerical schemes will result in linear algebraic equations [Atluri and Shen (2002); Cazzani, Garusi, Tralli and Atluri (2005); Chen, Fu and Qin (2010); Chen, Kao, and Chen (2009); Chen and Syong (2010); Divo and Kassab (2005); Gu, Young and Fan (2009); Han and Atluri (2004); Hon, Ling and Liew (2005); Hu, Young and Fan (2008); Jiang and Wu (2009); Liu (2007); Liu, Long and Li (2008); Marin (2009); Marin and Karageorghis (2009); Reutskiy (2005); Vavourakis and Polyzos (2007); Young, Chen and Wong (2005); Young, Tsai, Lin and Chen (2006)]. In contrary, the numerical algorithms for solving NAEs are very seldom. The most well-known numerical algorithms for solving NAEs are the Newton-like methods. Unfortunately, the Newton-like methods are usually sensitive to the initial guesses and the computational cost for calculating the inverse of Jacobian matrix is very expensive in every iteration step.

Recently, three algorithms, which can avoid the calculation of inverse of the Jacobian matrix, are proposed to efficiently deal with the NAEs. The first one is the fictitious time integration method (FTIM) [Liu (2008b); Liu (2009a); Liu (2009b); Liu (2009c); Liu (2009d); Liu and Atluri (2008a); Liu and Atluri (2008b); Liu and Atluri (2008c); Liu and Atluri (2009)], the second is the SHM [Liu, Yeih, Kuo and Atluri (2009)], and the third is the modified Newton method [Atluri, Liu and Kuo (2009)]. In the FTIM, the NAEs are transformed to the system of ordinary differential equations (ODEs) by introducing a fictitious time. Then, the ODEs can be integrated numerically to find the solutions of the original NAEs. The numerical procedure is very simple and converges very fast. Since the fictitious time is introduced, this algorithm can solve the ill-posed problems without any regularization [Chi, Yeih and Liu (2009)]. In addition, Ku, Yeih, Liu and Chi (2009) proposed a

new time-like function to fasten the convergence of the original FTIM. Although the FTIM performs well in solving NAEs, the numbers of equations and unknowns must be the same, which is not very flexible from the viewpoint of numerical simulations.

On the other hand, the SHM also transforms the NAEs to ODEs by introducing a scalar function and a fictitious time. Then, the ODEs will be numerically integrated to obtain the solutions of the NAEs. Motivated by the vector homotopy method, a scalar homotopy function is used to derive the evolution equation in SHM. Consequently, the SHM can keep the merits of the vector homotopy method, which is originated from Davidenko (1953). Due to the characteristic of global convergence, the SHM is insensitive to the initial guess of the numerical iterations. Hence, the restart scheme can be adopted to shorten the computational time. It is numerically proved that the SHM with the restart scheme can efficiently obtain the numerical solutions of the NAEs [Liu, Yeih, Kuo and Atluri (2009)]. In addition, the numbers of equations and unknowns can be different, which is very attractive in comparing with the vector homotopy method, the Newton-like methods and the FTIM. During the numerical implementation, the calculation of the inverse of Jacobian matrix can be avoided, which can reduce the computational cost in simulations. Besides, in the numerical experiments by Liu, Yeih, Kuo and Atluri (2009), the efficiency of SHM is better than the FTIM. Therefore, we will adopt the SHM, which is very stable and efficient in solving NAEs, for analyzing the nonlinear obstacle problems in this study.

In this paper, the NCP, which is used to describe the nonlinear obstacle problem, is discretized by the FDM with the aid of the NCP-function. Then, the resultant NAEs will be solved by the SHM with a global convergence. In addition, the restart scheme will be adopted to increase the efficiency of SHM in numerically integrating the ODEs. Once the evolutionary process of the SHM reaches the stopping criterion, the solutions of the resultant NAEs would be obtained. After a brief introduction of the motivation of this study, the nonlinear obstacle problems and the scalar homotopy method will be described. Then, several numerical examples will be provided to validate the proposed numerical scheme. Several factors will be examined through a series of numerical experiments to show the efficiency, stability and consistency of the proposed method. Finally, there are some conclusions that will be drawn according to the performances of the numerical experiments.

2 Non-Linear Obstacle Problems

One of the applications of the non-linear obstacle problems is to find the equilibrium position of an elastic string, u(x). The boundary of the elastic string, x = 0 and x = 4, is fixed and the equilibrium positions are lying above an obstacle which

is described by a given function, $\phi(x)$. A schematic diagram for this elastic string is depicted in Fig. 1. The equilibrium position should satisfy the following conditions:

$$u(0) = 0, (1)$$

$$u(4) = 0, (2)$$

$$u'(p_1) = \phi'(p_1),$$
 (3)

$$u'(p_2) = \phi'(p_2),$$
 (4)

$$u(x) = \phi(x) \text{ for } p_1 \le x \le p_2, \tag{5}$$

$$u''(x) = 0 \text{ for } 0 < x < p_1 \text{ or } p_2 < x < 4,$$
 (6)

where Eqs. (1) and (2) represent the fixed boundary condition. p_1 and p_2 are two endpoints when the elastic string and the obstacle coincide. Because the positions for p_1 and p_2 are unknown in prior, the numerical computation for such problem is very difficult. In order to avoid the computation for p_1 and p_2 , the above formulation can be reformulated as the NCP,

$$u(x) \ge \phi(x) \text{ for } 0 \le x \le 4,\tag{7}$$

$$u''(x) \le 0 \text{ for } 0 \le x \le 4,$$
 (8)

$$[u(x) - \phi(x)]u''(x) = 0 \text{ for } 0 \le x \le 4.$$
(9)

Eqs. (7)-(9) together with the boundary conditions in Eqs. (1) and (2) are equivalent to Eqs. (1)-(6). In this formulation, it does not need to find the positions of p_1 and p_2 explicitly. Unfortunately, due to the existence of inequalities in Eqs. (7) and (8), the numerical simulation for Eqs. (7)-(9) is still very difficult.

By adopting the Fischer-Burmeister NCP-function [Fischer (1992); Liu (2008a)], the system of Eqs. (7)-(9), can be converted to the following form:

$$\sqrt{(u(x) - \phi(x))^2 + (-u''(x))^2} - [(u(x) - \phi(x)) + (-u''(x))] = 0, \tag{10}$$

where the solution of Eq. (10) is equivalent to the solution of Eqs. (7)-(9), and vice versa. Since the formulation of the obstacle problem is transformed to an equality in Eq. (10), the FDM is adopted to discretize Eq. (10),

$$\sqrt{(u_i - \phi_i)^2 + \left(-\frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}\right)^2 - \left[u_i - \phi_i - \frac{u_{i+1} - 2u_i + u_{i-1}}{(\Delta x)^2}\right]} = 0,$$

$$i = 2, 3, ..., n - 1, \quad (11)$$

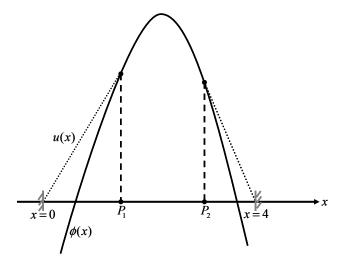


Figure 1: The schematic diagram for obstacle problem.

where *n* nodes are uniformly distributed from x = 0 to x = 4. Δx is the distance between two neighbor nodes. $u_i = u(x_i)$ and $\phi_i = \phi(x_i)$ are the positions of elastic string and obstacle at $x = x_i$. The two boundary conditions in Eqs. (1) and (2) can be written as

$$u_1 = 0, (12)$$

$$u_n = 0. (13)$$

After the FDM discretization and the use of NCP-function, the formulation of the obstacle problem becomes a system of NAEs in Eqs. (11)-(13). In this section, the formulation for one-dimensional problem is introduced. Similarly, the formulation for two-dimensional problem can be also derived by the same method. In the following section, the SHM will be introduced to solve the resultant NAEs.

3 Scalar Homotopy Method

We consider the system of NAEs from Eq. (11),

$$F_i(x_2, x_3, x_4, \dots, x_{n-1}) = 0, \quad i = 2, 3, 4, \dots, n-1,$$
 (14)

where we will use $\mathbf{x} := (x_2, x_3, x_4,, x_{n-1})^T$ and $\mathbf{F} := (F_2, F_3, F_4,, F_{n-1})^T$ to represent the vectors. In the homotopy theory, a path from the solution of a given function to the desired solution will be constructed continuously. Similar with the

vector homotopy, a scalar function, which is similar with the one proposed by Liu, Yeih, Kuo and Atluri (2009), is introduced,

$$h(\mathbf{x},t) = (1-t) \|\mathbf{F}(\mathbf{x}_0)\|^2 - \|\mathbf{F}(\mathbf{x})\|^2 = 0,$$
 (15)

where \mathbf{x}_0 is the initial value of \mathbf{x} at t = 0. For $t \in [0, 1]$, we have to analyze Eq. (15). When t = 0, it can be found that the scalar function is zero,

$$h(\mathbf{x}_0, t = 0) = \|\mathbf{F}(\mathbf{x}_0)\|^2 - \|\mathbf{F}(\mathbf{x}_0)\|^2 = 0.$$
(16)

Similarly, when t = 1, the scalar function will become:

$$h(\mathbf{x}, 1) = -\|\mathbf{F}(\mathbf{x})\|^2 = 0 \to F_i = 0, \ i = 2, 3, ..., n - 1.$$
 (17)

Therefore, when t = 1, the solution of the NAEs will be obtained. In order to satisfy Eq. (15) along the path, a consistency equation should be satisfied,

$$\frac{\partial h}{\partial t} + \frac{\partial h}{\partial \mathbf{x}} \cdot \frac{d\mathbf{x}}{dt} = 0. \tag{18}$$

From the theory of plasticity, we will note that $\frac{d\mathbf{x}}{dt}$ should be parallel to the gradient of the scalar function. Thus, Liu, Yeih, Kuo and Atluri (2009) proposed to use the following function:

$$\frac{d\mathbf{x}}{dt} = -q\frac{\partial h}{\partial \mathbf{x}}.\tag{19}$$

By substituted Eq. (19) into Eq. (18), we can acquire the following expression:

$$q = \frac{\frac{\partial h}{\partial t}}{\left\|\frac{\partial h}{\partial \mathbf{x}}\right\|^2}.$$
 (20)

Then, the above equation is substituted into Eq. (19) to derive the ODEs in SHM:

$$\frac{d\mathbf{x}}{dt} = -\frac{\frac{\partial h}{\partial t}}{\left\|\frac{\partial h}{\partial \mathbf{x}}\right\|^2} \frac{\partial h}{\partial \mathbf{x}},\tag{21}$$

where

$$\frac{\partial h}{\partial t} = -\|\mathbf{F}(\mathbf{x}_0)\|^2,\tag{22}$$

$$\frac{\partial h}{\partial \mathbf{x}} = -2\mathbf{B}^T \mathbf{F},\tag{23}$$

in which $\mathbf{B} := \frac{\partial \mathbf{F}}{\partial \mathbf{x}}$ is the Jacobian matrix of the NAEs.

Eq. (21) is the equation for an evolutionary process in the SHM and will be numerically integrated to obtain the solution of the NAEs. From the derivation of Eq. (21), it can be found that the calculation of the inverse of Jacobian matrix does not appear. For simplicity, we adopt the explicit Euler method to numerically integrate Eq. (21),

$$\mathbf{x}^{k+1} = \mathbf{x}^k - \Delta t \frac{\left(\frac{\partial h}{\partial t}\right)^k}{\left\|\left(\frac{\partial h}{\partial \mathbf{x}}\right)^k\right\|^2} \left(\frac{\partial h}{\partial \mathbf{x}}\right)^k,\tag{24}$$

where Δt is the time increment. The superscripts k and k+1 denote the k^{th} and the $(k+1)^{th}$ time steps.

Theoretically speaking, the solutions of NAEs can be acquired when *t* is equal to 1. If so, the satisfaction of consistency equation (18) should be kept rigorously during the numerical integration. Thus, a very small time increment will be required and the slowly convergent rate of SHM is almost the same with the vector homotopy method. Instead of using extremely small time increment, the restart method can be used to increase the convergence rate [Liu, Yeih, Kuo and Atluri (2009)]. The reason that the restart method can work is due to the global convergence of the SHM and more detailed explanations can refer to Liu, Yeih, Kuo and Atluri (2009).

By using the restart method, an adequate time increment can be used. The solution at t=1 surely is not the convergent solution of NAEs after the numerical integration. Then, the solution at t=1 will be assumed as the initial condition and the integration will be redid. The procedure can be repeated until the convergent solution is obtained. In this study, the convergence will be guaranteed if the following equation is satisfied,

$$\frac{\left\|\mathbf{F}\left(\mathbf{x}^{k}\right)\right\|^{2}}{ne} \le cri,\tag{25}$$

where *ne* is the number of equations and *cri* is the stopping criterion.

4 Numerical Results and Comparisons

In the following sections, four examples will be provided to validate the proposed scheme for dealing with the obstacle problems. Two of them are one-dimensional

problems and the others are two-dimensional problems. Besides, the influence of some factors, such as the number of nodes, the time increment and the initial guess, on the accuracy of the results will be examined by a series of numerical experiments.

4.1 Example 1

The first example is to find the equilibrium position of an elastic cable which is influenced by an obstacle, $\phi(x) = 1 - (x - 2.2)^2$. The formulation of this problem is [Billups and Murty (2000); Liu (2008a)]

$$u(x) - \phi(x) \ge 0 \quad \forall x \in [0, 4], \tag{26}$$

$$-u''(x) \ge 0 \quad \forall x \in [0,4],\tag{27}$$

$$[u(x) - \phi(x)]u''(x) = 0 \quad \forall x \in [0, 4], \tag{28}$$

$$u(0) = u(4) = 0. (29)$$

Unless otherwise specified, the following parameters are used in this example: n = 41, $\Delta t = 0.1$, initial guess $\left[Ig = 2\sin\left(\frac{\pi x}{4}\right)\right]$ and $cri = 10^{-5}$. In Fig. 2, we used 21, 41, 61, 81 and 101 nodes to solve the problem. The equilibrium positions of the elastic cable and the obstacle are plotted in this figure and those numerical solutions are very close to each other. The results are very similar with the solution by Liu (2008a). Therefore, we tabulated these results in Table 1 to examine the solutions. Furthermore, the results from different time increments are depicted in Fig. 3. It can be found that convergent solutions are almost identical by four different time increments. In Fig. 4, the solutions by different initial guesses are demonstrated. From Figs. (2)-(4), it is proved that the proposed scheme is very stable and accurate with respect to the number of nodes, time increments and initial guesses.

4.2 Example 2

Next, we consider the following problem [Liu (2008a)]:

$$\phi(x) - u(x) \ge 0 \quad \forall x \in [0, 2], \tag{30}$$

$$u''(x) + 5u(x) - u^{2}(x) \ge 0 \quad \forall x \in [0, 2],$$
 (31)

$$[\phi(x) - u(x)] [u''(x) + 5u(x) - u^{2}(x)] = 0 \quad \forall x \in [0, 2],$$
(32)

$$u(0) = u(2) = 0, (33)$$

where the obstacle is described by $\phi(x) = 1 + (x - 1)^2$.

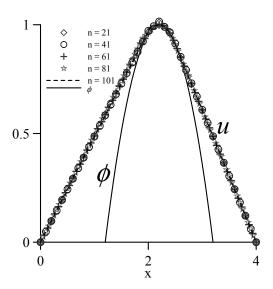


Figure 2: The profiles of solutions by different numbers of nodes for example 1.

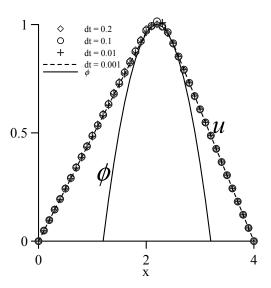


Figure 3: The profiles of solutions by different time increments for example 1.

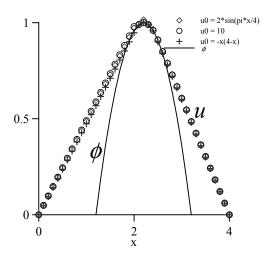


Figure 4: The profiles of solutions by different initial guesses for example 1.

X	n=21	n=41	n=61	n=81	n=101	φ
1.0	4.83E-01	4.86E-01	4.89E-01	4.94E-01	4.87E-01	-4.40E-01
1.2	5.80E-01	5.83E-01	5.87E-01	5.93E-01	5.84E-01	0.00E+00
1.4	6.77E-01	6.80E-01	6.84E-01	6.91E-01	6.82E-01	3.60E-01
1.6	7.73E-01	7.78E-01	7.82E-01	7.90E-01	7.78E-01	6.40E-01
1.8	8.70E-01	8.75E-01	8.80E-01	8.89E-01	8.75E-01	8.40E-01
2.0	9.66E-01	9.72E-01	9.61E-01	9.65E-01	9.71E-01	9.60E-01
2.2	1.01E+00	1.01E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
2.4	9.67E-01	9.65E-01	9.60E-01	9.60E-01	9.60E-01	9.60E-01
2.6	8.46E-01	8.52E-01	8.50E-01	8.49E-01	8.49E-01	8.40E-01
2.8	7.25E-01	7.31E-01	7.29E-01	7.27E-01	7.28E-01	6.40E-01
3.0	6.05E-01	6.09F-01	6.07F-01	6.06F-01	6.06F-01	3.60F-01

Table 1: The numerical solutions by different numbers of nodes for example 1.

In the numerical experiments, the following parameters are used: n=21, $\Delta t=0.1$, $Ig=2\sin\left(\frac{\pi x}{2}\right)$ and $cri=10^{-6}$. The numerical solutions by different numbers of nodes are shown in Fig. 5. The numerical results are almost identical in this figure. Therefore, the results are tabulated in Table 2 to see the consistency of the solutions. Besides, the results by different time increments and different initial guesses are demonstrated in Figs. 6 and 7. The consistency, stability and global convergence of the proposed methods are proved numerically again in the second example.

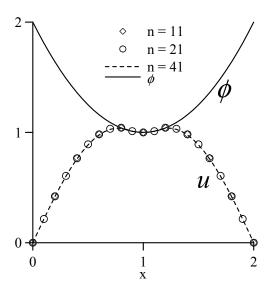


Figure 5: The profiles of solutions by different number of nodes for example 2.

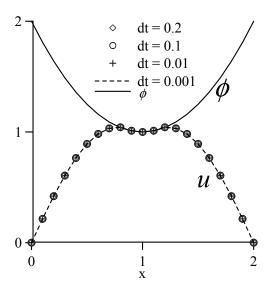


Figure 6: The profiles of solutions by different time increments for example 2.

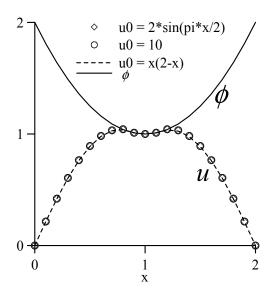


Figure 7: The profiles of solutions by different initial guesses for example 2.

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X	n=11	n=21	n=41	n=61	ϕ
0.2	4.23E-01	4.20E-01	4.18E-01	4.18E-01	1.64E+00
0.4	7.69E-01	7.65E-01	7.61E-01	7.61E-01	1.36E+00
0.6	9.85E-01	9.82E-01	9.77E-01	9.77E-01	1.16E+00
0.8	1.04E+00	1.04E+00	1.04E+00	1.04E+00	1.04E+00
1.0	1.00E+00	1.00E+00	1.00E+00	1.00E+00	1.00E+00
1.2	1.04E+00	1.04E+00	1.04E+00	1.04E+00	1.04E+00
1.4	9.85E-01	9.82E-01	9.77E-01	9.77E-01	1.16E+00
1.6	7.69E-01	7.65E-01	7.61E-01	7.61E-01	1.36E+00
1.8	4.23E-01	4.20E-01	4.18E-01	4.18E-01	1.64E+00

4.3 Example 3

For the third example, we consider a two-dimensional problem [Korman, Leung, Stojanovic (1990); Liu (2008a)]:

$$\left(1+x^2y^2\right)\frac{\partial^2 u}{\partial x^2} + \left(1+\frac{y}{2}\right)\frac{\partial^2 u}{\partial y^2} + 15u - u^2 \ge 0,\tag{34}$$

$$10 - u \ge 0,\tag{35}$$

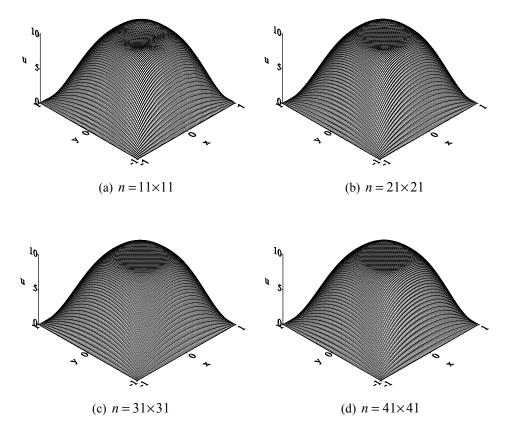


Figure 8: The distributions of solutions by different numbers of nodes for example 3.

$$\[\left(1 + x^2 y^2 \right) \frac{\partial^2 u}{\partial x^2} + \left(1 + \frac{y}{2} \right) \frac{\partial^2 u}{\partial y^2} + 15u - u^2 \] [10 - u] = 0, \tag{36}$$

where the computational domain is a square: $\Omega = (-1,1) \times (-1,1)$.

The following parameters are used in this example: $\Delta t = 0.1$, Ig = 10 and $cri = 10^{-3}$. The results by different numbers of nodes are demonstrated in Fig. 8. In this figure, four different numbers of computational nodes are used and the solutions are very close to each other. Besides, the results are similar with the solution by Liu (2008a). In order to check the results carefully, the profiles of u(x,y) at y=0 along x axis are depicted in Fig. 9. From this figure, we can find that the solutions converge fast even by using a few of nodes. In addition, the influence of the obstacle, $\phi(x,y) = 10$, can be found clearly. The influences of time increment and initial guess on the accuracy of solutions are identical with the previous examples.

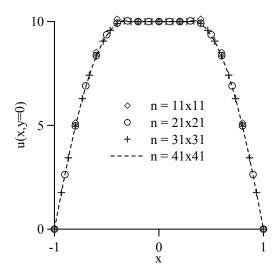


Figure 9: The profiles of solutions at y = 0 along x axis for example 3.

Therefore, the solutions and comparisons are omitted for the sake of simplicity.

4.4 Example 4

For the fourth example, the following NCP is considered [Zhang (2001)]:

$$-\Delta u \ge -50 \quad (x, y) \in \Omega \tag{37}$$

$$u \ge -0.5 \quad (x, y) \in \Omega \tag{38}$$

$$(-\Delta u + 50)(u + 0.5) = 0 \quad (x, y) \in \Omega$$
(39)

$$u = 0 \quad (x, y) \in \Gamma \tag{40}$$

where the computational domain is a unit square: $\Omega = (0,1) \times (0,1)$.

The following parameters are used in this example: $\Delta t = 0.1$, Ig = -0.5 and $cri = 10^{-5}$. The convergent solutions for different numbers of computational nodes are shown in Fig. 10. The solutions are very similar with each other and the results by Zhang (2001). In order to examine the results carefully, the profiles of the solutions at y = 0.5 along x axis are depicted in Fig. 11. In the figure, it can be found that the solution will become better if more nodes are used. In addition, the influence of the obstacle, $\phi(x,y) = -0.5$, can be discovered easily.

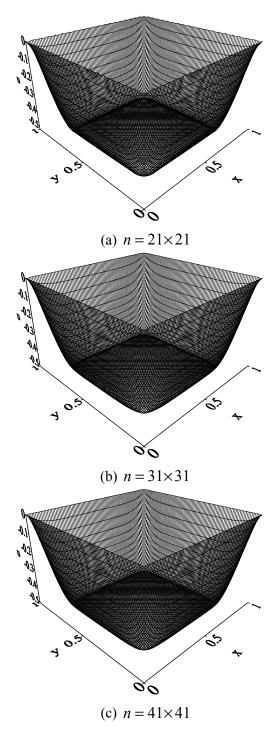


Figure 10: The distributions of solutions by different numbers of nodes for example 4.

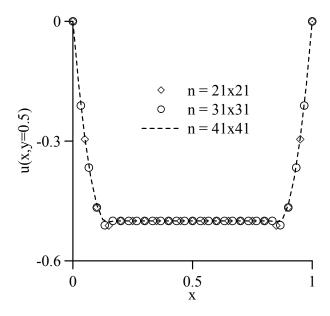


Figure 11: The profiles of solutions at y = 0.5 along x axis for example 4.

5 Conclusions

The combination of SHM and FDM is proposed to analyze the nonlinear obstacle problems. The NCP, used to formulate the obstacle problems, is transformed to NAEs by using the NCP-function and the FDM. Then, the resultant NAEs are solved by the SHM, which is globally convergent. The SHM, derived by introducing a scalar homotopy and a fictitious time, retains the merits of the vector homotopy method. In addition, the restart method is adopted to fasten the convergence rate of the SHM. Four examples are provided to validate the proposed scheme. Besides, different numbers of nodes, different time increments and different initial guesses are used to examine the characteristics of the proposed scheme. From those results and comparisons, the efficiency, stability and consistency of the proposed method are shown evidently. Therefore, it can be believed that the combination of SHM and FDM can form an efficient and stable numerical scheme for solving the nonlinear obstacle problems.

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