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A Time-Marching Algorithm for Solving Non-Linear Obstacle Problems with the Aid of an NCP-Function

Chein-Shan Liu[1]

Abstract: Proposed is a time-marching algorithm to solve a nonlinear system of complementarity equations: $P_i(x_j) \geq 0,\ Q_i(x_j) \geq 0,\ P_i(x_j)Q_i(x_j) = 0,\ i, j = 1, \ldots, n$, resulting from a discretization of nonlinear obstacle problem. We transform the above nonlinear complementarity problem (NCP) into a nonlinear algebraic equations (NAEs) system: $F_i(x_j) = 0$ with the aid of the Fischer-Burmeister NCP-function. Such NAEs are semi-smooth, highly nonlinear and usually implicit, being hard to handle by the Newton-like method. Instead of, a first-order system of ODEs is derived through a fictitious time equation. The time-stepping equations are obtained by applying a numerical integration on the resultant ODEs, which are derivative-free and do not need the inverse of any matrix. The computational cost is thus greatly reduced. The numerical examples of Bratu, von Karman and other elliptic equations are used to demonstrate that the new fictitious time integration method (FTIM) is highly efficient to calculate the obstacle problems.

Keyword: Nonlinear Obstacle Problem, Nonlinear complementarity problem, Nonlinear algebraic equations, Iterative method, Elliptic equations, Fictitious time integration method (FTIM)

1 Introduction

Let $\Omega \in \mathbb{R}^d$ be a given domain. The obstacle problem consists in finding the equilibrium position of an elastic membrane subject to an external force f and an obstacle φ; see, e.g., Rodrigues (1987). Hence, the infinite-dimensional problem is to minimize the total energy

$$E(u) = \int_\Omega \left(\frac{1}{2} \|\nabla u\|^2 - fu \right) dx, \tag{1}$$

such that u belongs to the following cone:

$$K = \{ v \in H_0^1(\Omega) | v \geq \varphi \text{ a.e. in } \Omega \}. \tag{2}$$

The optimality conditions for this optimization problem lead to a variational inequality of finding an element $u \in K$, such that

$$\int_\Omega \nabla u \cdot \nabla (v - u) dx \geq \int_\Omega f(v-u) dx, \ \ \forall v \in K. \tag{3}$$

Under a weak regularity condition, this is equivalent to a complementarity formulation:

$$-\Delta u \geq f, \ \ \forall x \in \Omega, \tag{4}$$

$$u \geq \varphi, \ \ \forall x \in \Omega, \tag{5}$$

$$(-\Delta u - f)(u - \varphi) = 0, \ \ \forall x \in \Omega, \tag{6}$$

$$u = 0, \ \ \forall x \in \partial\Omega. \tag{7}$$

The coincidence set of this obstacle problem is defined as

$$\omega = \{ x \in \Omega | u(x) = \varphi(x) \}, \tag{8}$$

and the boundary of ω is a free boundary not known a priori [Freidman (1982); Freidman and Phillips (1984); Kinderlehrer and Stampacchia (1980)]. The set ω is rather complex as shown by Caffarelli (1998).

We should stress that the obstacle problem in Eqs. (4)-(7) is much difficult than the Poisson problem of $\Delta u = -f$, of which there are many numerical studies, like as, Wordelman, Aluru and Ravaioli (2000), Tsai, Lin, Young and Atluri (2006), and Tsai (2008).

[1] Department of Mechanical and Mechatronic Engineering, Computation and Simulation Center, Taiwan Ocean University, Keelung, Taiwan. E-mail: csliu@mail.ntou.edu.tw

The quadratic programming and linear complementarity methods for solving certain simple obstacle problems have been well documented. Obstacle problems that lead to mixed NCPs include the obstacle Bratu problem [Hoppe and Mittelmann (1989); Miersemann and Mittelmann (1989)], and the obstacle von Karman problem [Yau and Gao (1992)]. Typically, these problems are formulated in an infinite-dimensional function space and their discretizations could easily lead to finite-dimensional problems of very large size. Numerical solution of the discretized obstacle Bratu problem is discussed by Chen and Mangasarian (1996), and several others.

Apart from the above variational inequalities problem of elliptic equation, there were rich sources for complementarity problems. A general complementarity problem is to find a solution $\mathbf{x} \in \mathbb{R}^n$ of the following complementary trios system:

$$\mathbf{P}(\mathbf{x}) \geq \mathbf{0}, \;\; \mathbf{Q}(\mathbf{x}) \geq \mathbf{0}, \;\; \mathbf{P}^{\mathrm{T}}\mathbf{Q} = 0, \tag{9}$$

where $\mathbf{P}, \mathbf{Q} \in \mathbb{R}^n$ denote vector functions with P_i and Q_i their components. Many applications from engineering sciences, economics, game theory etc. lead to problems of this kind; see Ferris and Pang (1997) for a survey. Most algorithms for the solution of complementarity problem are based on a suitable reformulation either as a system of algebraic equations, as an optimization problem, or as a fixed-point problem, etc. We refer the interested reader to the survey paper by Harker and Pang (1990) for the basic ideas of some algorithms. In fact, many of these reformulations can be obtained for more general mixed complementarity problem. The new method in this paper is based on a reformulation of the complementarity problem (9) as a system of nonlinear algebraic equations (NAEs):

$$\mathbf{F}(\mathbf{x}) = \mathbf{0}, \tag{10}$$

where $\mathbf{F} \in \mathbb{R}^n$ is defined componentwise by

$$F_i(\mathbf{x}) := \phi(P_i(\mathbf{x}), Q_i(\mathbf{x})) \tag{11}$$

for some mapping $\phi : \mathbb{R}^2 \mapsto \mathbb{R}$ having the property of

$$\phi(a,b) = 0 \Leftrightarrow a \geq 0, \;\; b \geq 0, \;\; ab = 0. \tag{12}$$

Clearly, this property guarantees that a vector $\mathbf{x} \in \mathbb{R}^n$ is a solution of the complementarity problem (9) if and only if $\mathbf{x}$ solves the equations system (10). Applying Newton's method to system (10) then leads to one class of semismooth methods; see Chen, Chen and Kanzow (2000), De Luca, Facchinei and Kanzow (1996, 2000), Facchinei and Kanzow (1997), Jiang, Fukushima, Qi and Sun (1998), Jiang and Qi (1997), Ulbrich (2001), Yamashita and Fukushima (1997), and Ito and Kunisch (2007) for some references. Depending on the choice of the mapping ϕ, different methods with different properties can be obtained. Some of these methods have been discussed in detail by Kanzow (2004).

Most semismooth methods have a very strong theoretical background and seem to be quite reliable and efficient also from a numerical point of view, at least when an exact Newton-type method is applied to the system (10). However, in the large-scale case, we may not be able to find the exact solution of the corresponding linearized equation. There are other methods to solve the NCPs, like as smoothing or non-smoothing Newton method [Qi and Sun (1993); Taji and Miyamoto (2002)], and homotopy method [Watson (1979)]. Usually, the resulting NAEs from the equivalent formulation of NCP-function are non-smooth, highly nonlinear as well as implicit, and it is desired to develop more efficient method to calculate the solutions.

For the following algebraic equations:

$$F_i(x_1, \ldots, x_n) = 0, \;\; i = 1, \ldots, n, \tag{13}$$

the Newton method is given by

$$\mathbf{x}_{k+1} = \mathbf{x}_k - [\mathbf{B}(\mathbf{x}_k)]^{-1}\mathbf{F}(\mathbf{x}_k), \tag{14}$$

where we use $\mathbf{x} := (x_1, \ldots, x_n)^{\mathrm{T}}$ and $\mathbf{F} := (F_1, \ldots, F_n)^{\mathrm{T}}$ to represent the vectors, and $\mathbf{B}$ is an $n \times n$ matrix with its ij-th component given by $\partial F_i / \partial x_j$.

Newton method has a great advantage that it is quadratically convergent, however, it still has some drawbacks. Some quasi-Newton methods are thus developed; see the discussions by Broyden (1965), Dennis (1971), Dennis and More (1974, 1977), and Spedicato and Huang (1997).

Davidenko (1953) has developed a new idea of homotopy method to solve Eq. (13) by numerically integrating

$$\dot{\mathbf{x}}(t) = -\mathbf{H}_{\mathbf{x}}^{-1}\mathbf{H}_t(\mathbf{x},t), \tag{15}$$

$$\mathbf{x}(0) = \mathbf{a}, \tag{16}$$

where $\mathbf{H}$ is a homotopic vector function, for example, $\mathbf{H} = (1-t)(\mathbf{x}-\mathbf{a}) + t\mathbf{F}(\mathbf{x})$, and $\mathbf{H}_{\mathbf{x}}$ and $\mathbf{H}_t$ are the partial derivatives of $\mathbf{H}$ with respect to $\mathbf{x}$ and t. This theory is later refined by Kellogg, Li and Yorke (1976), Chow, Mallet-Paret and Yorke (1978), Li and Yorke (1980), and Li (1997). At the same time, Hirsch and Smale (1979) also derived a continuous Newton method governed by the following differential equation:

$$\dot{\mathbf{x}}(t) = -\mathbf{B}^{-1}(\mathbf{x})\mathbf{F}(\mathbf{x}), \tag{17}$$

$$\mathbf{x}(0) = \mathbf{a}. \tag{18}$$

It can be seen that the ODEs in Eqs. (15) and (17) are difficult to calculate, because they all include an inverse matrix. The monographs by Allgower and Georg (1990) and Deuflhard (2004) are devoted to the continuation methods for solving NAEs. Below we will develop a new ODEs system, which are equivalent to the original equation (13).

2 A fictitious time integration approach

2.1 Transformation of NCP into an algebraic equations system

The NCP under some conditions can be transformed into other mathematically equivalent problems, like as algebraic equations and optimization equations. Let x be a solution of an NCP, that is, $x \geq 0$, $F(x) \geq 0$, and $xF(x) = 0$. Obviously, it is equivalent to that x is a solution of the minimum problem: $\min(x, F(x)) = 0$. The function ϕ is said to be an NCP-function: if $\phi : \mathbb{R}^2 \mapsto \mathbb{R}$ and $\phi(a,b) = 0$ iff $a \geq 0,\ b \geq 0,\ ab = 0$.

In addition the minimum function there are many other NCP-functions. In this study we will employ the Fischer-Burmeister [Fischer (1992)] NCP-function:

$$\phi_{\text{FB}}(a,b) = \sqrt{a^2+b^2} - (a+b). \tag{19}$$

Thus for a general NCP of Eq. (9), we write it to be

$$F_i = \phi_{\text{FB}}(P_i, Q_i) = \sqrt{P_i^2 + Q_i^2} - (P_i + Q_i) = 0, \quad i = 1, \ldots, n. \tag{20}$$

Up to now one of the most powerful approaches that has been studied intensively is to reformulate the NCP as a system of NAEs [Mangasarian (1976); Yamashita and Fukushima (1997)], or as an unconstrained minimization problem [Mangasarian and Solodov (1993); Yamashita and Fukushima (1995); Chen, Gao and Pan (2008)]. Such a function that can constitute an equivalent unconstrained minimization problem for the NCP is called a merit function. In other words, a merit function is a function whose global minima are coincident with the solutions of the original NCP. For constructing a merit function, the class of NCP-functions serves an important role. Some more depth studies of the NCP-functions and merit functions can refer the papers by Facchinei and Soares (1997), Sun and Qi (1999), Chen (2006, 2007), and Chen and Pan (2008).

2.2 Transforming into an ODEs system

Recently, derivative-free methods have attracted some attentions as can be seen from Yamada, Yamashita and Fukushima (2000), Chen (2006), Chen and Pan (2008), and Chen, Gao and Pan (2008), which do not require the computation of derivatives of the given functions $\mathbf{F}$. Derivative-free methods, taking advantages of particular properties of a merit function, are suitable for problems where the derivatives of $\mathbf{F}$ are not available or expensive.

In the present paper we propose another derivative-free method to solve the NCPs. Let us consider the following transformation:

$$y_i(t) = (1+t)x_i, \quad i = 1, \ldots, n, \tag{21}$$

and multiply a coefficient $-\nu \neq 0$ in Eq. (20):

$$0 = -\nu F_i(x_1, \ldots, x_n). \tag{22}$$

Using Eq. (21) we have

$$0 = -\nu F_i\left(\frac{y_1}{1+t}, \ldots, \frac{y_n}{1+t}\right). \tag{23}$$

Recalling that $\dot{y}_i = x_i$ by Eq. (21), and adding it on both the sides of the above equation we obtain

$$\dot{y}_i = x_i - \nu F_i\left(\frac{y_1}{1+t},\ldots,\frac{y_n}{1+t}\right). \tag{24}$$

Then, by using $x_i = y_i/(1+t)$, we can change Eq. (20) into an ODEs system:

$$\dot{y}_i = \frac{y_i}{1+t} - \nu F_i\left(\frac{y_1}{1+t},\ldots,\frac{y_n}{1+t}\right). \tag{25}$$

Finally, multiplying each equation by the integrating factor $1/(1+t)$ and using Eq. (21) again we obtain

$$\dot{x}_i = \frac{-\nu}{1+t}F_i(x_1,\ldots,x_n),\ \ i = 1,\ldots,n. \tag{26}$$

It can be seen that this ODEs system is nonautonomous and is much simpler than those in Eqs. (15) and (17).

Furthermore, in terms of a logarithmic time scale

$$\tau = \ln(1+t), \tag{27}$$

Eq. (26) can be recast to a neater form:

$$\frac{dx_i}{d\tau} = -\nu F_i(x_1,\ldots,x_n),\ \ i = 1,\ldots,n. \tag{28}$$

The above idea is first proposed by Liu (2008a) to treat an inverse Sturm-Liouville problem by transforming an ODE into a PDE. Then, Liu and his coworkers [Liu (2008b, 2008c); Liu, Chang, Chang and Chen (2008)] extended this idea to develop new method for estimating parameters in the inverse vibration problems. Recently, Liu and Atluri (2008) have cleverly employed the technique of fictitious time integration method (FTIM) to solve large system of NAEs, and showed that high performance can be achieved by using the FTIM.

Eq. (21) is not the unique way to transform the algebraic equations (20) into the ODEs. We can adopt

$$y_i(t) = q(t)x_i,\ \ i = 1,\ldots,n, \tag{29}$$

and a similar derivation leads to

$$\dot{x}_i = \frac{-\nu}{q(t)}F_i(x_1,\ldots,x_n),\ \ i = 1,\ldots,n. \tag{30}$$

The requirements of $q(t)$ are differentiable and $q(0) = 1$. A special case is $q(t) = 1$ and $\nu = -1$, and then we have

$$\dot{x}_i = F_i(x_1,\ldots,x_n). \tag{31}$$

Deuflhard (2004) has called the above equation a pseudo-transient continuation method. However, this equation is hard to work and usually leads to wrong solutions of the roots of $F_i = 0$.

From Eq. (28) we understand that the so-called steady state must be considered in the logarithmic time scale $\tau = \ln(1+t)$, because this equation is no more a nonautonomous one as Eq. (26) is. In the logarithmic time scale, if the motion of x_i approaches a steady state, i.e., $dx_i/d\tau = 0$, then the roots are found. In this paper we focus on using Eq. (26) as our tool to compute the solutions of NCPs. This is the most simple choice of $q(t) = 1+t$ to meet the just mentioned requirements of $q(t)$. However, other choices are possible if they can provide more better behavior than the present one.

2.3 GPS for ODEs system

We can write Eq. (26) as

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x},t),\ \ \mathbf{x} \in \mathbb{R}^n,\ \ t > 0, \tag{32}$$

where $f_i = -\nu F_i/(1+t)$ is the i-th component of $\mathbf{f}$.

Group-preserving scheme (GPS) can preserve the internal symmetry group of the considered ODEs system. Although we do not know previously the symmetry group of differential equations system, Liu (2001) has embedded it into an augmented differential system, which concerns with not only the evolution of state variables themselves but also the evolution of the magnitude of the state variables vector. Let us note that

$$\|\mathbf{x}\| = \sqrt{\mathbf{x}^{\mathrm{T}}\mathbf{x}} = \sqrt{\mathbf{x}\cdot\mathbf{x}}, \tag{33}$$

where the dot between two n-dimensional vectors denotes their inner product. Taking the derivatives of both the sides of Eq. (33) with respect to t, we have

$$\frac{d\|\mathbf{x}\|}{dt} = \frac{(\dot{\mathbf{x}})^{\mathrm{T}}\mathbf{x}}{\sqrt{\mathbf{x}^{\mathrm{T}}\mathbf{x}}}. \tag{34}$$

Then, by using Eqs. (32) and (33) we can derive

$$\frac{d\|\mathbf{x}\|}{dt}=\frac{\mathbf{f}^{\mathrm{T}}\mathbf{x}}{\|\mathbf{x}\|}. \tag{35}$$

It is interesting that Eqs. (32) and (35) can be combined together into a simple matrix equation:

$$\frac{d}{dt}\begin{bmatrix}\mathbf{x}\\ \|\mathbf{x}\|\end{bmatrix}=\begin{bmatrix}\mathbf{0}_{n\times n} & \frac{\mathbf{f}(\mathbf{x},t)}{\|\mathbf{x}\|}\\ \frac{\mathbf{f}^{\mathrm{T}}(\mathbf{x},t)}{\|\mathbf{x}\|} & 0\end{bmatrix}\begin{bmatrix}\mathbf{x}\\ \|\mathbf{x}\|\end{bmatrix}. \tag{36}$$

It is obvious that the first row in Eq. (36) is the same as the original equation (32), but the inclusion of the second row in Eq. (36) gives us a Minkowskian structure of the augmented state variables of $\mathbf{X}:=(\mathbf{x}^{\mathrm{T}},\|\mathbf{x}\|)^{\mathrm{T}}$, which satisfies the cone condition:

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X}=0, \tag{37}$$

where

$$\mathbf{g}=\begin{bmatrix}\mathbf{I}_n & \mathbf{0}_{n\times 1}\\ \mathbf{0}_{1\times n} & -1\end{bmatrix} \tag{38}$$

is a Minkowski metric, and $\mathbf{I}_n$ is the identity matrix of order n. In terms of $(\mathbf{x},\|\mathbf{x}\|)$, Eq. (37) becomes

$$\mathbf{X}^{\mathrm{T}}\mathbf{g}\mathbf{X}=\mathbf{x}\cdot\mathbf{x}-\|\mathbf{x}\|^2=\|\mathbf{x}\|^2-\|\mathbf{x}\|^2=0. \tag{39}$$

It follows from the definition given in Eq. (33), and thus Eq. (37) is a natural result.

Consequently, we have an $n+1$-dimensional augmented system:

$$\dot{\mathbf{X}}=\mathbf{A}\mathbf{X} \tag{40}$$

with a constraint (37), where

$$\mathbf{A}:=\begin{bmatrix}\mathbf{0}_{n\times n} & \frac{\mathbf{f}(\mathbf{x},t)}{\|\mathbf{x}\|}\\ \frac{\mathbf{f}^{\mathrm{T}}(\mathbf{x},t)}{\|\mathbf{x}\|} & 0\end{bmatrix}, \tag{41}$$

satisfying

$$\mathbf{A}^{\mathrm{T}}\mathbf{g}+\mathbf{g}\mathbf{A}=\mathbf{0}, \tag{42}$$

is a Lie algebra $so(n,1)$ of the proper orthochronous Lorentz group $SO_o(n,1)$. This fact prompts us to devise the group-preserving scheme (GPS), whose discretized mapping $\mathbf{G}$ must exactly preserve the following properties:

$$\mathbf{G}^{\mathrm{T}}\mathbf{g}\mathbf{G}=\mathbf{g}, \tag{43}$$

$$\det\mathbf{G}=1, \tag{44}$$

$$G_0^0>0, \tag{45}$$

where G_0^0 is the 00-th component of $\mathbf{G}$.

Although the dimension of the new system is raised one more, it has been shown that the new system permits a GPS given as follows [Liu (2001)]:

$$\mathbf{X}_{k+1}=\mathbf{G}(k)\mathbf{X}_k, \tag{46}$$

where $\mathbf{X}_k$ denotes the numerical value of $\mathbf{X}$ at t_k, and $\mathbf{G}(k)\in SO_o(n,1)$ is the group value of $\mathbf{G}$ at t_k. If $\mathbf{G}(k)$ satisfies the properties in Eqs. (43)-(45), then $\mathbf{X}_k$ satisfies the cone condition in Eq. (37).

The Lie group can be generated from $\mathbf{A}\in so(n,1)$ by an exponential mapping,

$$\mathbf{G}(k)=\exp[h\mathbf{A}(k)]=\begin{bmatrix}\mathbf{I}_n+\frac{(a_k-1)}{\|\mathbf{f}_k\|^2}\mathbf{f}_k\mathbf{f}_k^{\mathrm{T}} & \frac{b_k\mathbf{f}_k}{\|\mathbf{f}_k\|}\\ \frac{b_k\mathbf{f}_k^{\mathrm{T}}}{\|\mathbf{f}_k\|} & a_k\end{bmatrix}, \tag{47}$$

where

$$a_k:=\cosh\left(\frac{h\|\mathbf{f}_k\|}{\|\mathbf{x}_k\|}\right), \tag{48}$$

$$b_k:=\sinh\left(\frac{h\|\mathbf{f}_k\|}{\|\mathbf{x}_k\|}\right). \tag{49}$$

Substituting Eq. (47) for $\mathbf{G}(k)$ into Eq. (46), we obtain

$$\mathbf{x}_{k+1}=\mathbf{x}_k+\eta_k\mathbf{f}_k, \tag{50}$$

$$\|\mathbf{x}_{k+1}\|=a_k\|\mathbf{x}_k\|+\frac{b_k}{\|\mathbf{f}_k\|}\mathbf{f}_k\cdot\mathbf{x}_k, \tag{51}$$

where

$$\eta_k:=\frac{b_k\|\mathbf{x}_k\|\|\mathbf{f}_k\|+(a_k-1)\mathbf{f}_k\cdot\mathbf{x}_k}{\|\mathbf{f}_k\|^2}. \tag{52}$$

This scheme is group properties preserved for all $h>0$, and is called the group-preserving scheme.

2.4 Numerical procedure

Starting from an initial value of $\mathbf{x}(0)$ which can be guessed in a rather free way, we employ the above GPS to integrate Eq. (32) from $t = 0$ to a selected final time t_f. In the numerical integration process we check the convergence of x_i at the k- and $k+1$-steps by

$$\sum_{i=1}^{n}(x_i^{k+1} - x_i^k)^2 \leq \varepsilon^2, \tag{53}$$

where ε is a selected criterion. If at a time $t_0 \leq t_f$ the above criterion is satisfied, then the solution of x_i is obtained. In practice, if a suitable t_f is selected we find that the numerical solution is also approached very well to the true solution, even the above convergent criterion is not satisfied. The coefficient ν introduced in Eq. (26) can increase the stability of numerical integration.

In particular we should emphasize that the present method is a new fictitious time integration method (FTIM), which can calculate the solution very stably and effectively. Below we give numerical examples of NCPs for obstacle problems to display some advantages of the present FTIM.

3 Numerical tests

Many obstacle problems in mathematical physics lead to nonlinear complementarity problems, which mainly focused on the determination of free boundaries. In this section we use one- and two-dimensional obstacle problems as numerical tests of our algorithm.

3.1 Example 1

An elastic cable is obstacled by a plane curve of the shape $\varphi(x) = 1-(x-2.2)^2$, and its two ends are fixed at two points $(0,0)$ and $(4,0)$. As shown in Fig. 1 there are two unknown points x_1 and x_2 at which the values of the elastic displacement u are the same as that obtained from φ by inserting the coordinates of x_1 and x_2. In the intervals of $[0,x_1]$ and $[x_2,4]$ the deformations of elastic cable are straight lines connected $(0,0)$ and $(x_1,\varphi(x_1))$ and $(x_2,\varphi(x_2))$ and $(4,0)$. The elastic displacement u satisfies

$$u(0) = u(4) = 0, \quad u(x) = \varphi(x), \quad \forall x \in [x_1,x_2], \tag{54}$$

$$u'(x_1) = \varphi'(x_1), \quad u'(x_2) = \varphi'(x_2), \tag{55}$$

$$u''(x) = 0, \quad 0 < x < x_1, \quad x_2 < x < 4. \tag{56}$$

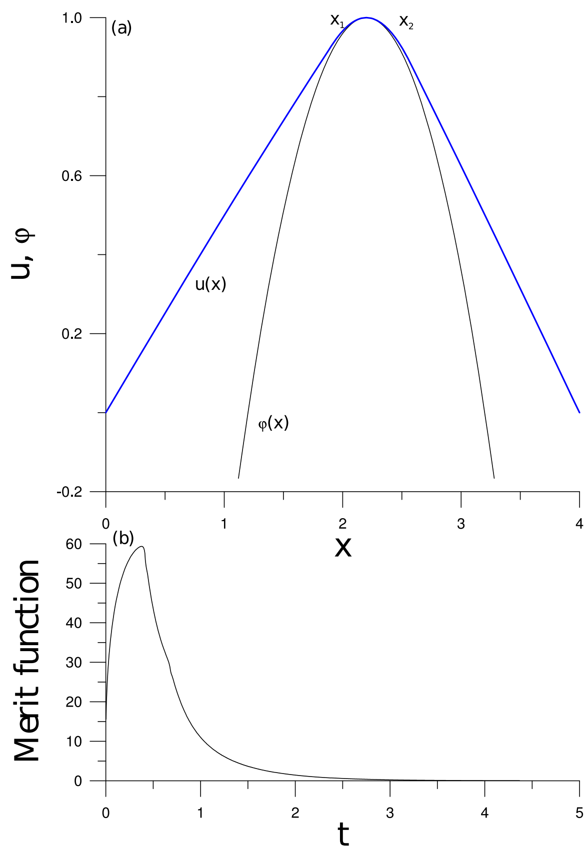

Figure 1: For Example 1 (a) the profiles of u and φ are plotted, very well matching the required inequalities, and (b) showing the convergent in terms of merit function.

Due to the unknown boundaries of x_1 and x_2, the above problem is hard to solve. In terms of complementary trios we can write [Billups and Murty (2000)]

$$u(x) - \varphi(x) \geq 0, \quad \forall x \in [0,4], \tag{57}$$

$$-u''(x) \geq 0, \quad \forall x \in [0,4], \tag{58}$$

$$[u(x) - \varphi(x)]u''(x) = 0, \quad \forall x \in [0,4], \tag{59}$$

where $u(x)$ is subjected to $u(0) = u(4) = 0$.

By introducing a finite difference discretization of u'' at the grid points we can obtain

$$u_i - \varphi_i \geq 0, \tag{60}$$

$$-\frac{1}{(\Delta x)^2}(u_{i+1} - 2u_i + u_{i-1}) \geq 0, \tag{61}$$

$$\frac{(u_i - \varphi_i)}{(\Delta x)^2}(u_{i+1} - 2u_i + u_{i-1}) = 0, \tag{62}$$

where $u_i = u(x_i)$, $\varphi_i = \varphi(x_i)$ and $x_i = i\Delta x = 4i/(n+1)$. Now, the governing ODEs are given by

$$\dot{u}_i = \frac{-\nu}{1+t}\left[\sqrt{\frac{1}{(\Delta x)^4}(u_{i+1} - 2u_i + u_{i-1})^2 + (u_i - \varphi_i)^2} + \frac{1}{(\Delta x)^2}(u_{i+1} - 2u_i + u_{i-1}) - u_i + \varphi_i\right]. \tag{63}$$

Under the following parameters: $n = 99$, $\nu = -0.5$, $\varepsilon = 10^{-4}$, and $h = 0.001$ and starting from an initial value of $u_i = 1$, the FTIM converges within 4369 steps, that is, the terminal time is $t_f = 4.369$. In Fig. 1(a) we plot the curves of u and φ. It can be seen that the present numerical result matches the above inequalities very well. Defining the merit function as $\sum_{i=1}^{n} F_i^2/2$, we plot its time history in Fig. 1(b), from which we can see that the new method after the first half time unit is convergent exponentially with time.

3.2 *Example 2*

Next we calculate the following obstacle problem:

$$\varphi(x) - u(x) \geq 0, \quad \forall x \in [0,2], \tag{64}$$

$$u''(x) + 5u(x) - u^2(x) \geq 0, \quad \forall x \in [0,2], \tag{65}$$

$$[\varphi(x) - u(x)][u''(x) + 5u(x) - u^2(x)] = 0, \quad \forall x \in [0,2], \tag{66}$$

where $u(x)$ is subjected to $u(0) = u(2) = 0$, and $\varphi(x) = 1 + (x-1)^2$.

Under the following parameters: $n = 59$, $\nu = 5$, $\varepsilon = 4 \times 10^{-6}$, and $h = 0.0001$ and starting from an initial value of $u_i = 2$, the FTIM converges within 19229 steps, that is, the terminal time is $t_f = 1.9229$. In Fig. 2 we plot the curves of u and φ respectively by thick and thin solid lines. It can be seen that the present numerical result is quite well.

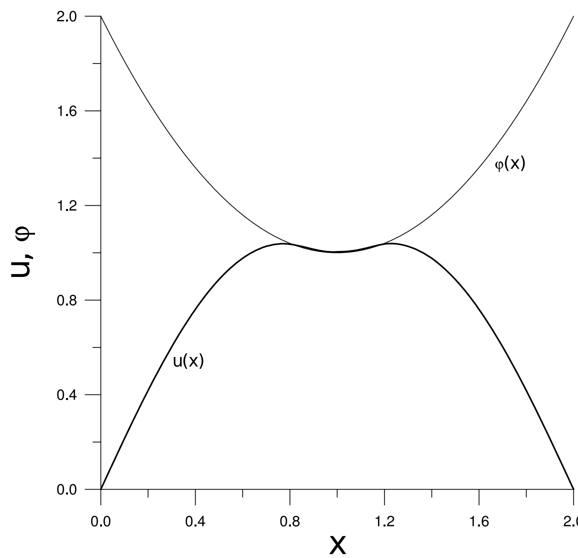

Figure 2: For Example 2 the profiles of u and φ are plotted, matching the required inequalities very well.

3.3 *Example 3*

In this example we apply the FTIM to solve the following free boundary value problem of nonlinear elliptic equation of a two-dimensional obstacle problem [Kanzow (2004)], known as the obstacle Bratu problem:

$$-\Delta u(x,y) + \lambda \exp[u(x,y)] \geq 0, \quad (x,y) \in \Omega = (0,1) \times (0,1), \tag{67}$$

$$u(x,y) - \varphi \geq 0, \quad (x,y) \in \Omega, \tag{68}$$

$$\{-\Delta u(x,y) + \lambda \exp[u(x,y)]\}\{u(x,y) - \varphi\} = 0, \quad (x,y) \in \Omega. \tag{69}$$

In Fig. 3 we plot three surfaces of $u(x,y)$ for three different $(\lambda, \varphi) = (2,-1.5)$, $(3,-3)$, $(1,-4)$, all starting from the initial values of $u_{ij} = 0.1$. Other parameters are fixed to be $\Delta x = \Delta y = 1/50$, $h = 0.001$, $\nu = -0.1$, and $\varepsilon = 10^{-4}$. For this problem there are multiple solutions; in Fig. 4 we plot the surfaces by starting from the initial values of

$u_{ij} = -1.5$ for the first case, $u_{ij} = -3$ for the second case, and $u_{ij} = -4$ for the third case. It can be seen that these solutions are larger than that in Fig. 3.

3.4 Example 4

In this example we apply the FTIM to solve the following two-dimensional obstacle problem [Korman, Leung and Stojanovic (1990)]:

$$(1+x^2y^2)\frac{\partial^2 u(x,y)}{\partial x^2} + \left(1+\frac{y}{2}\right)\frac{\partial^2 u(x,y)}{\partial y^2} + 15u(x,y) - u^2(x,y) \geq 0, \quad (70)$$

$$10 - u(x,y) \geq 0, \quad (71)$$

$$\left\{(1+x^2y^2)\frac{\partial^2 u(x,y)}{\partial x^2} + \left(1+\frac{y}{2}\right)\frac{\partial^2 u(x,y)}{\partial y^2} + 15u(x,y) - u^2(x,y)\right\}\{10-u(x,y)\} = 0, \quad (72)$$

where $(x,y) \in \Omega = (-1,1)\times(-1,1)$. In Fig. 5 we plot the surface of $u(x,y)$. In the calculation of this example we have used $\Delta x = \Delta y = 2/30$, $h = 0.0001$, $\nu = 5$, and before $t_f = 1$ the iterations are convergent under a criterion of $\varepsilon = 10^{-4}$. The initial conditions of $u_{ij} = 10$ are used. The computational cost is very saving with a CPU time smaller than one second by using the ASUS A6000 Note Book.

3.5 Example 5

Then, we calculate the following obstacle problem of von Karman [Ferris and Pang (1997)]:

$$u''''(x) - 5[u'(x)]^2u''(x) \geq f(x), \quad \forall x \in [-1,1], \quad (73)$$

$$u(x) \geq \varphi(x), \quad \forall x \in [-1,1], \quad (74)$$

$$\{u''''(x) - 5[u'(x)]^2u''(x) - f(x)\}\{u(x)-\varphi(x)\} = 0, \quad \forall x \in [-1,1], \quad (75)$$

where $u(x)$ is subjected to the clamped boundary conditions $u(-1) = u(1) = -0.5$ and $u'(-1) = u'(1) = 0$. Here, $f(x) = 1+(x-1)^2$ and $\varphi(x) = 1-2x^2$. Under the following parameters: $n = 49$,

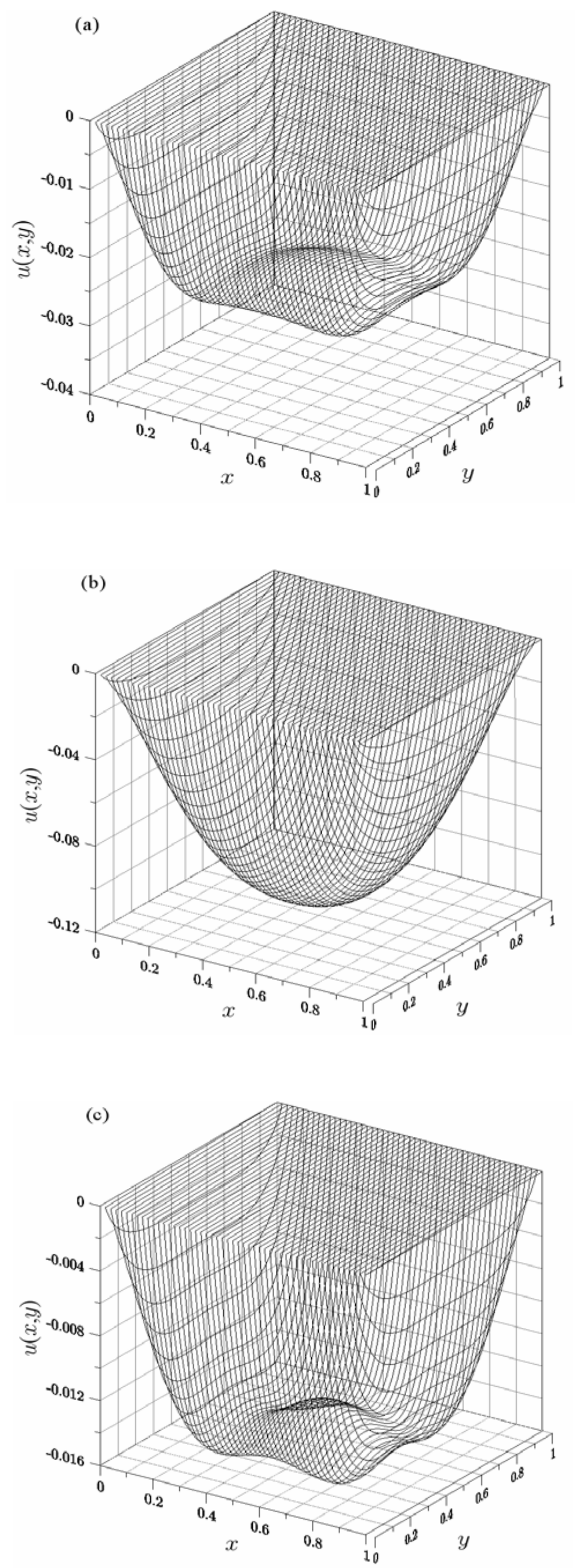

Figure 3: Smaller solutions for two-dimensional Bratu obstacle problems with different parameters.

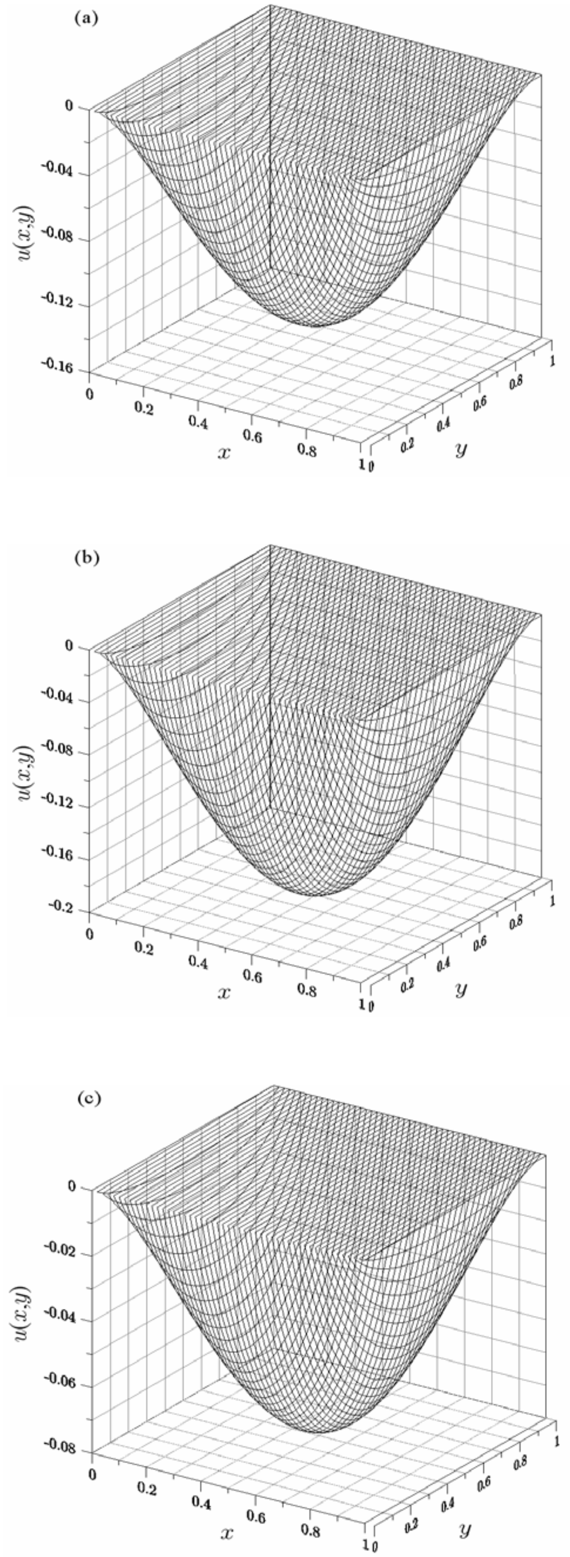

Figure 4: Larger solutions for two-dimensional Bratu obstacle problems with different parameters.

$\nu = -0.01$, $\varepsilon = 2 \times 10^{-6}$, and $h = 0.00001$ and starting from an initial value of $u_i = -1$, the FTIM converges within 337 steps, that is, the terminal time is $t_f = 0.00337$. In Fig. 6 we plot the curves of u and φ respectively by thick and thin solid lines. It can be seen that the present numerical result matches the above inequalities very well.

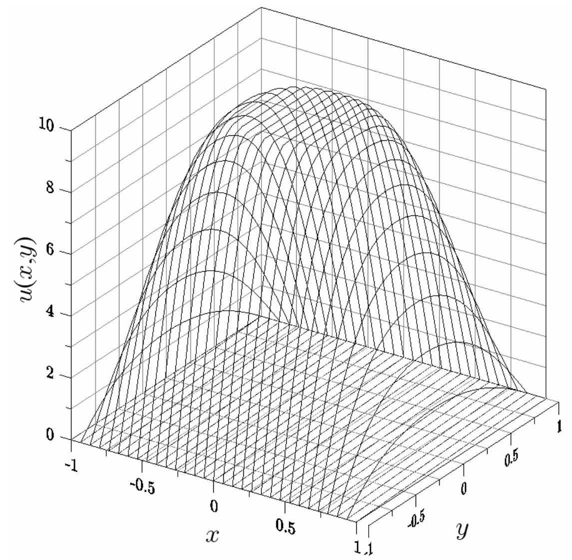

Figure 5: The solution for a two-dimensional elliptic obstacle problem.

3.6 Example 6

Finally, we come to an algebraic NCP as investigated by Kojima and Shindo (1986):

$$\begin{aligned} & x_1 \geq 0, \\ & F_1 = 3x_1^2 + 2x_1x_2 + 2x_2^2 + x_3 + 3x_4 - 6 \geq 0, \\ & x_1F_1 = 0, \end{aligned} \tag{76}$$

$$\begin{aligned} & x_2 \geq 0, \\ & F_2 = 2x_1^2 + x_1 + x_2^2 + 10x_3 + 2x_4 - 2 \geq 0, \\ & x_2F_2 = 0, \end{aligned} \tag{77}$$

$$\begin{aligned} & x_3 \geq 0, \\ & F_3 = 3x_1^2 + x_1x_2 + 2x_2^2 + 2x_3 + 9x_4 - 9 \geq 0, \\ & x_3F_3 = 0, \end{aligned} \tag{78}$$

$$\begin{aligned} & x_4 \geq 0, \\ & F_4 = x_1^2 + 3x_2^2 + 2x_3 + 3x_4 - 3 \geq 0, \\ & x_4F_4 = 0. \end{aligned} \tag{79}$$

In our FTIM we use the GPS to solve the following nonlinear ODEs:

$$\dot{x}_1 = \frac{-\nu}{1+t}\left[\sqrt{F_1^2+x_1^2}-F_1-x_1\right], \tag{80}$$

$$\dot{x}_2 = \frac{-\nu}{1+t}\left[\sqrt{F_2^2+x_2^2}-F_2-x_2\right], \tag{81}$$

$$\dot{x}_3 = \frac{-\nu}{1+t}\left[\sqrt{F_3^2+x_3^2}-F_3-x_3\right], \tag{82}$$

$$\dot{x}_4 = \frac{-\nu}{1+t}\left[\sqrt{F_4^2+x_4^2}-F_4-x_4\right]. \tag{83}$$

By using $h = 0.01$, $\nu = -20$ and $\varepsilon = 10^{-10}$, and starting from $(x_1,x_2,x_3,x_4) = (0.5,0.2,-0.1,1)$ we calculate the solution as $(x_1,x_2,x_3,x_4) = (1.224745, 5.4 \times 10^{-10}, -1.34 \times 10^{-10}, 0.5)$ within 154 steps. The numerical errors as compared with the exact solution of $(x_1,x_2,x_3,x_4) = (\sqrt{6}/2,0,0,0.5)$ are smaller than 10^{-10}. Similarly, starting from $(x_1,x_2,x_3,x_4) = (0.5,0.2,0.1,1)$ we calculate the solution as $(x_1,x_2,x_3,x_4) = (1, 5.96\times10^{-16}, 3, 1.09\times10^{-12})$ within 386 steps. The numerical errors as compared with the exact solution of $(x_1,x_2,x_3,x_4) = (1,0,3,0)$ are smaller than 10^{-12}. The computations are finished smaller than one second of CPU time.

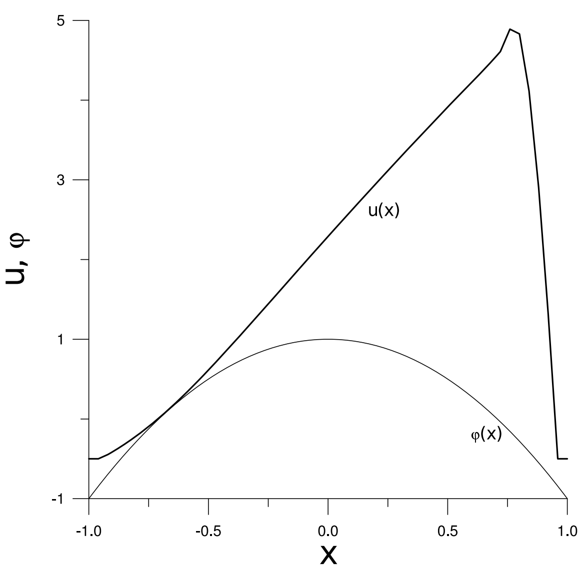

Figure 6: For Example 5 the profiles of u and φ are plotted, well matching of the required inequalities.

4 Conclusions

In this paper we only consider the Fischer-Burmeister NCP-function as a bridge to transform the NCP to an equivalent system of NAEs. Since the work of Newton, iterative algorithms are developed by many researchers extending to continuous type by an extra ad hoc artificial time. However, those ODEs required the derivative of **F** and some variants of the Jacobian matrix associated with **F**. This is difficult to handle the NCPs because the resulting algebraic equations are nonsmooth. The present paper was wit enough to transform the nonsmooth NAEs into an evolutionary equations system by introducing a fictitious time, without resorting on the derivative of **F**. The coefficient ν may be positive or negative dependent on problems at hand; suitable ν can increase the stability of numerical integration and speeds up the convergence. Undoubtedly, the present FTIM can work very effectively and accurately for the solutions of nonlinear obstacle problems. Several numerical examples of obstacle problems in one- or two-dimensional spaces were worked out. Because no derivative and no inverse of matrix are required, the present method is very time saving.

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