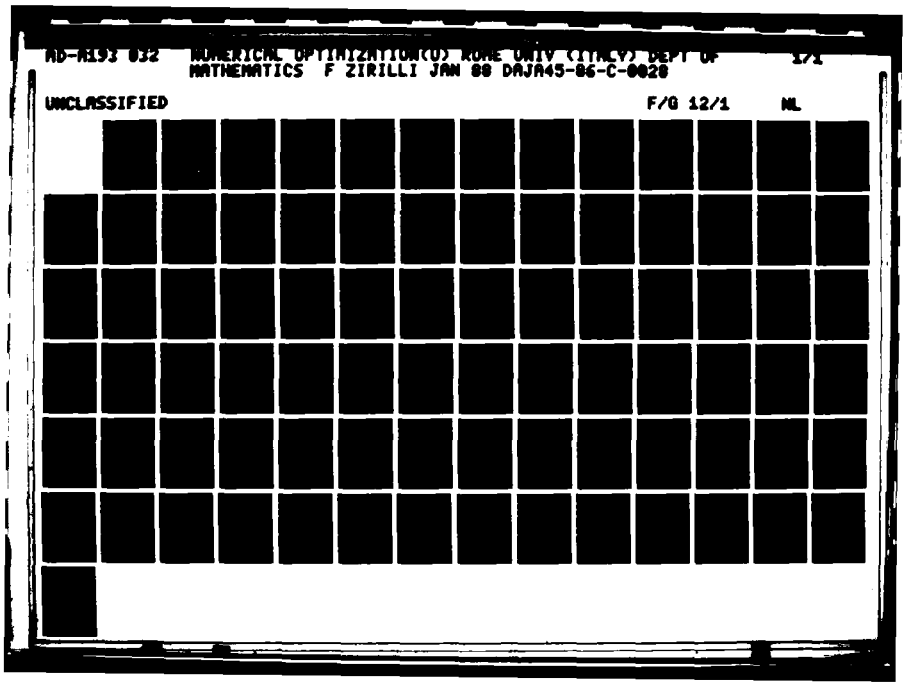
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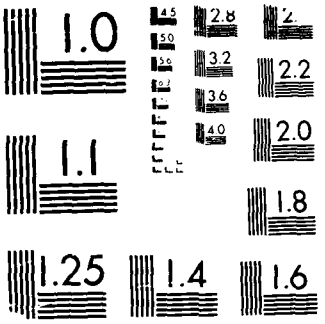

AD 1

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Contractor: Università di Roma "La Sapienza"
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INDEX

1. Statement of scientific work done during the reporting period

The first objective we pursued was to build some test problems in the area of linear and nonlinear complementarity problems in order to be able to verify the practical value of our algorithms before submitting them to a detailed mathematical analysis. A large variety of problems of different difficulty belongs to the area of linear and nonlinear complementarity; to start our investigation we have considered three problems that come from the discretization of variational inequalities of mathematical physics (see Appendix 4.1). The first two problems are linear complementarity problems; the third one is a nonlinear complementarity problem. The corresponding continuous problems involve ordinary or partial differential operators so that when discretized a large number (up to a few thousand) independent variables can be considered. For these problems existence and uniqueness of the solution can be proved; moreover, they have some intrinsic interest given their mathematical physics interpretation. A FORTRAN computer code implementing these three complementarity problems has been written.

The complementarity problems considered above have been translated into a system of nonlinear equations (see Appendix 4.2). On the resulting systems of nonlinear equations the algorithm DAFNE (ref. [1], [2], [3]) based on the use of ordinary differential equations and the algorithm SIGMA (ref. [4], [5], [6]) based on the use of stochastic differential equations have been used.

For a system of nonlinear equations with n-independent variables DAFNE solves an $n \times n$ linear system at each step so that with n on the order of one thousand the computational cost of the linear algebra is substantial. To avoid this difficulty an inexact-DAFNE algorithm in the spirit of [7] has been proposed (see Appendix 4.3) and tested on the test problems with satisfactory results.

At the moment the performance of SIGMA on problems with hundreds of independent variables is unsatisfactory.

2. Research plans for the immediate future

In the immediate future we plan to pursue the following objectives:

(i) carry out a mathematical analysis of the inexact-DAFNE algorithm considered in Appendix 4.3

(ii) investigate how to adapt the SIGMA algorithm to work on problems involving thousands of independent variables

(iii) study the behavior of our methods on linear and nonlinear complementarity problems where existence and uniqueness of solution is not guaranteed.

3. Administrative actions

The following investigators are working on the contract:

(i) Francesco Zirilli
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During the period September 1, 1986 - December 31, 1986 Francesco Zirilli will be visiting:

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4. Appendices

Appendix 4.1. Test Problems

Let $\mathbb{R}^n$ be the n-dimensional real euclidean space, let $\underline{x} = (x_1, x_2 \ldots, x_n)^T \in \mathbb{R}^n$, and for $\underline{x}, \underline{y} \in \mathbb{R}^n$ let $\left\langle \underline{x}, \underline{y} \right\rangle = \underline{x}^T \underline{y} = \sum_{i=1}^{n} x_i y_i$ be the scalar product between $\underline{x}$ and $\underline{y}$ and $||\underline{x}|| = \left\langle \underline{x}, \underline{x} \right\rangle^{1/2}$ the euclidean norm of $\underline{x}$.

The first problem considered arises as a one-dimensional free-boundary problem in the lubrication theory of an infinite journal bearing, i.e. a rotating cylinder separated from a bearing surface by a thin film of lubricating fluid ref [8]. The finite-difference approximation used by Cryer in [8] leads to

Problem A (called Problem 3D by Cryer): Find $\underline{x}, \underline{w} \in \mathbb{R}^n$ such that

$$\underline{w} = \underline{q} + M\underline{x}, \quad \underline{w} \geq \underline{0}, \quad \underline{x} \geq \underline{0}, \tag{4.1.1}$$

$$\left\langle \underline{w}, \underline{x} \right\rangle = 0, \tag{4.1.2}$$

where $M = ((M_{ij}))$, $i, j = 1, 2, \ldots, n$ is an $n \times n$ matrix with elements M_{ij} given by

$$\begin{aligned} M_{ij} &= -(H_{i+1/2})^3, && \text{if } j = i+1, \\ M_{ij} &= [(H_{i+1/2})^3 + (H_{i-1/2})^3], && \text{if } j = i, \\ M_{ij} &= -(H_{i-1/2})^3, && \text{if } j = i-1, \\ M_{ij} &= 0, && \textit{otherwise} \end{aligned} \tag{4.1.3}$$

and $\underline{q} = (q_1, q_2, \ldots, q_n)^T$ is a vector with elements q_i given by

$$q_i = \frac{T}{n+1} [H_{i+1/2} - H_{i-1/2}], \quad i = 1, 2, \ldots n \tag{4.1.4}$$

where

$$H_{i \pm 1/2} = H((i \pm 1/2) \frac{T}{n+1}) \tag{4.1.5}$$

and the function $H(y)$ is given by

$$
\begin{aligned}
&g_L(y) = \tfrac{1}{2}(Y-y)^2, \\
&g_R(y) = \tfrac{1}{2}(W-y)^2, \qquad \text{if } y < W, \\
&g_R(y) = 0, \qquad \text{if } y \geq W, \\
&g_D(x) = Y^2/2 - (Y^2 - W^2)(x/2X), \\
&g_U(x) = 0, \\
&r_{ij} = -Dx\,Dy + \delta_{i1}\,a\,g_L(j\,Dy) + \delta_{i n_x}\,a\,g_R(j\,Dy) \\
&\qquad\qquad + \delta_{ij}(1/a)\,g_D(i\,Dx) + \delta_{n_y j}(1/a)\,g_U(i\,Dx), \\
&\qquad i = 1, 2, \ldots, n_x, \qquad j = 1, 2, \ldots, n_y .
\end{aligned}
$$

The elements $q_1, q_2, \ldots, q_n$ of $\underline{q}$ are given by

$$q_k = r_{ij}, \quad \textit{with} \quad k = (j-1)\,n_x + i \tag{4.1.10}$$

Our last problem, which is defined below, can be interpreted as a finite-difference approximation of a nonlinear variational inequality.

Problem C: Find $\underline{x}, \underline{w} \in \mathbb{R}^n$ such that

$$\underline{w} = M\underline{x} + pu2{,}let(\underline{x}) + \underline{q}, \quad \underline{w} \geq 0, \quad \underline{x} \geq 0 \tag{4.1.15}$$

$$\left\langle \underline{w}, \underline{x} \right\rangle = 0 \tag{4.1.16}$$

The problem dimension n, the quantities Dx, Dy and the matrix M are defined as in problem B, given n_x, n_y, X, Y. The nonlinear term $\underline{p}(\underline{x})$ is a vector in $\mathbb{R}^n$ with components $p_i = x_i^3$, $i = 1, \ldots, n$. The vector $\underline{q} = (q_1, q_2, \ldots, q_n)^T$ is defined by equation (4.1.10) where $r_{ij} = Dx\,Dy \sin(2\pi\, iDx/X)$, $i = 1, 2, \ldots, n_x$, $j = 1, 2, \ldots, n_y$.

Appendix 4.2. The system of nonlinear equations

Problem 1 (Linear complementarity problem). Let M be an $n \times n$ real matrix and $\underline{q} \in \mathbb{R}^n$. Find $\underline{w}, \underline{z} \in \mathbb{R}^n$ such that

$$\underline{w} = \underline{q} + M\underline{z}, \quad \underline{w} \geq \underline{0}, \ \underline{z} \geq \underline{0}, \tag{4.2.1}$$

$$\left\langle \underline{w}, \underline{z} \right\rangle = 0, \tag{4.2.2}$$

where $\underline{w} \geq \underline{0}$ and $\underline{z} \geq \underline{0}$ mean that each component of $\underline{w}$ and $\underline{z}$ is greater than or equal to zero.

Problem 2 (Nonlinear complementarity problem). Let $\underline{f}: \mathbb{R}^n \to \mathbb{R}^n$ be a given map. Find $\underline{z} \in \mathbb{R}^n$ such that

$$\underline{z} \geq \underline{0}, \quad \underline{f}(\underline{z}) \geq \underline{0} \tag{4.2.3}$$

$$\left\langle \underline{f}(\underline{z}), \underline{z} \right\rangle = 0. \tag{4.2.4}$$

A complementarity problem can be reformulated as a problem of solving a system of nonlinear equations, as follows.

Let $\Theta: \mathbb{R} \to \mathbb{R}$ a strictly increasing function such that $\Theta(0) = 0$. As it was shown by Mangasarian (ref. [10]), $\underline{z}$ solves the nonlinear complementarity problem (4.2.3), (4.2.4) (Problem 2) if and only if $\underline{z}$ solves the system of nonlinear equations

$$g_i(\underline{z}) \equiv \Theta(|f_i(\underline{z}) - z_i|) - \Theta(f_i(\underline{z})) - \Theta(z_i) = 0, \quad i = 1, 2, \ldots, n, \tag{4.2.5}$$

where $\underline{z} = (z_1, z_2, \ldots, z_n)^T$ and $\underline{f} = (f_1, f_2, \ldots, f_n)^T$.

Problem 1 is a special case of (4.2.5) when $\underline{f}(\underline{z}) = \underline{q} + M\underline{z}$.

Appendix 4.3. The inexact-DAFNE algorithm

In the following we choose $\Theta(t) = t/2$ so that the nonlinear complementarity problem (Problem 2) is equivalent to

$$\underline{g}(\underline{x}) = \underline{0} \tag{4.3.1}$$

where $\underline{g}(\underline{x}) = (g_1(\underline{x}), g_2(\underline{x}), \ldots, g_n(\underline{x}))^T \in \mathbb{R}^n$ and

$$\begin{aligned} g_i(\underline{x}) &= \tfrac{1}{2}\left(|f_i(\underline{x}) - x_i| - f_i(\underline{x}) - x_i\right) \\ &= -\min\left(x_i, f_i(\underline{x})\right), \qquad i = 1, 2, \ldots, n . \end{aligned}$$

For the linear complementarity problem (Problem 1), it is enough to choose $\underline{f}(\underline{x}) = \underline{q} + M\underline{x}$.

We note that $\underline{g}(\underline{x})$ is not everywhere-differentiable; however if $\underline{x}^*$ is a non-degenerate solution of the complementarity problem (Problem 2), i.e. such that $\underline{x}^* + \underline{f}(\underline{x}^*) > 0$, then, in a neighbourhood of $\underline{x}^*$, $\underline{g}(\underline{x})$ has at least the same regularity properties of $\underline{f}(\underline{x})$. Moreover, as shown by Mangasarian [10], if all the principal minors of the jacobian of $\underline{f}(\underline{x})$ are non-singular at $\underline{x}^*$ then the jacobian of $\underline{g}$ at $\underline{x}^*$ is non-singular.

We consider now the problem of solving the system of simultaneous equations (4.3.1) and assume that $\underline{f}$ is regular enough to justify what follows. We define

$$G(\underline{x}) = \underline{g}^T(\underline{x}) \cdot \underline{g}(\underline{x}) = \sum_{j=1}^{n} g_j^2(\underline{x}); \tag{4.3.2}$$

it is easy to see that $\underline{x}^*$ is an isolated solution of (4.3.1) if and only if $G(\underline{x}^*) = 0$ and $\underline{x}^*$ is an isolated (global) minimizer of $G(\underline{x})$.

Incerti, Parisi and Zirilli [11] proposed the following second-order system of ordinary differential equations

$$\mu \frac{d^2\underline{x}}{dt^2} = -\beta D \frac{d\underline{x}}{dt} - \nabla G(\underline{x}), \tag{4.3.3}$$

where μ, β are positive constants, D is an $n \times n$ symmetric positive matrix and where ∇G is the gradient of G with respect to x. The equations (4.3.3) represent Newton's second law (*mass* $\times$ *acceleration* $=$ *force*) for a particle of mass μ moving in $\mathbb{R}^n$ subject to the force $-\nabla G$ given by the potential G and to the force $-\beta D \frac{d\underline{x}}{dt}$. Since $\beta > 0$ the force $-\beta D \frac{d\underline{x}}{dt}$ is a dissipa-

tive force.

If $\underline{x}^*$ is such that $G(\underline{x}^*)=0$, $\underline{x}^*$ is a (global) minimizer of $g(\underline{x})$, and $\underline{x}(t)\equiv\underline{x}^*$ is a solution of (4.3.3). Consider the Cauchy data:

$$\underline{x}(0)=\underline{x}_0, \qquad \frac{d\underline{x}}{dt}(0)=\underline{v}_0, \tag{4.3.4}$$

and let $\underline{x}(t,\underline{x}_0,\underline{v}_0)$ be the solution of the initial value problem (4.3.3), (4.3.4). Then if $\beta>0$ under some mild assumptions on $G(\underline{x})$ it can be shown that if $||\underline{x}_0-\underline{x}^*||$ and $||\underline{v}_0||$ are small enough then

$$\lim_{t\to 0}||\underline{x}(t,\underline{x}_0,\underline{v}_0)-\underline{x}^*||=0, \tag{4.3.5}$$

so that we try to solve the original problem (4.3.1) by computing the solution $\underline{x}(t,\underline{x}_0,\underline{v}_0)$ of (4.3.3) (4.3.4) for suitable $\underline{x}_0$, $\underline{v}_0$.

The performance of this method to solve the nonlinear system (4.3.1) is greatly dependent on the numerical scheme used to solve (4.3.3), (4.3.4).

Several numerical schemes to solve (4.3.3), (4.3.4) have been considered by Aluffi, Incerti, Zirilli [12], [13] and the simplest linearly implicit A-stable scheme among those proposed by Lambert and Sigurdsson [14] has been chosen. Finally, for the corresponding algorithms to solve the nonlinear system (4.3.1) Zirilli [1] carried out a local convergence and rate of convergence analysis.

Let $\underline{y}\in\mathbb{R}^m$, $\underline{\phi}(t,\underline{y})$ be a regular function from $\mathbb{R}\times\mathbb{R}^m$ to $\mathbb{R}^m$ and consider the initial value problem:

$$\frac{d\underline{y}}{dt}=\underline{\phi}(t,\underline{y}), \tag{4.3.6}$$

$$\underline{y}(0)=\underline{y}_0. \tag{4.3.7}$$

The class of the linear k-step finite-differences schemes with variable matrix coefficients introduced by Lambert and Sigurdsson [14] to solve (4.3.6), (4.3.7) is given by the formula:

$$\sum_{j=0}^{k}(a_j^{(0)}I+\sum_{r=1}^{s}h^r a_j^{(r)}Q_i^r)\underline{y}_{i+j} = h\sum_{j=0}^{k}(b_j^{(0)}I+\sum_{r=1}^{s-1}h^r b_j^{(r)}Q_i^r)\underline{\phi}_{i+j}, \tag{4.3.8}$$

where $h > 0$ is the time integration step-length, $t_i = ih$, $\underline{\phi}_i(t_i, \underline{y}_i)$. Moreover Q_i is an $m \times m$ matrix such that, for all i, $||Q_i|| \leq q = constant$ and $a_k^{(0)} I + \sum_{r=1}^{s} h^r a_k^{(r)} Q_i^r$ is non-singular. We note that when

$$a_j^{(r)} = 0\,, \quad r = 1, 2, ..., s\,, \quad j = 0, 1, ..., k$$

and

$$b_j^{(r)} = 0\,, \quad r = 1, 2, ..., s-1\,, \quad j = 0, 1, ..., k$$

the class (4.3.8) reduces to the class of linear k-step methods with scalar coefficients.

Some of the methods contained in (4.3.8) are A-stable in the sense of Dahlquist and linearly implicit; that is, to compute a step only a linear system must be solved. The simplest method with these properties is given by the formula

$$(I - h\Phi_i)(\underline{y}_{i+1} - \underline{y}_i) = h\underline{\phi}_i\,, \tag{4.3.9}$$

where $\Phi_i = \dfrac{\partial \phi_i}{\partial \underline{y}}(t_i, \underline{y}_i)$ is the jacobian of $\underline{\phi}$ with respect to $\underline{y}$.

After rewriting (4.3.3) as a first order system:

$$\begin{aligned} \frac{d\underline{x}}{dt} &= \underline{v}\,, \\ \frac{d\underline{v}}{dt} &= -\frac{\beta}{\mu} D\underline{v} - \frac{1}{\mu} \nabla G(\underline{x})\,, \end{aligned} \tag{4.3.10}$$

formula (4.3.9) with variable time-integration step-length h_i (i.e. $t_i = \sum_{j=0}^{i-1} h_j$, $i = 1, 2, ..., t_0 = 0$) is applied to compute the trajectory of (4.3.3), (4.3.4).

In (4.3.10) the map $\underline{\phi}$ is given by

$$\underline{\phi}: \begin{bmatrix} \underline{x} \\ \underline{v} \end{bmatrix} \to \begin{bmatrix} \underline{v} \\ -\dfrac{\beta}{\mu} D\underline{v} - \dfrac{1}{\mu} \nabla G(\underline{x}) \end{bmatrix} \tag{4.3.11}$$

so that its jacobian Φ is given by

$$\Phi = \begin{bmatrix} 0 & I \\ -\dfrac{1}{\mu} L(\underline{x}) & -\dfrac{\beta}{\mu} D \end{bmatrix} \tag{4.3.12}$$

where

$$L(\underline{x}) = 2[J^T(\underline{x})J(\underline{x}) + \sum_{i=1}^{n} g_i(\underline{x})\, H_i(\underline{x})]\,, \tag{4.3.13}$$

$J(\underline{x}) = \dfrac{\partial \underline{g}}{\partial \underline{x}}$ is the jacobian of $\underline{g}$ with respect to x and $H(x)$ i the hessian of $g(x)$.

We consider here the algorithm implemented in the DAFNE package (Aluffi-Pentini, Parisi, Zirilli, [2], [3]). Let

$$\underline{s}_i = \underline{x}_{i+1} - \underline{x}_i\,, \qquad i = 0, 1, 2, \cdots \tag{4.3.14}$$

Applying (4.3.9) to (4.3.10) we obtain after some simple algebra

$$[L_i + \frac{1}{h_i}(\frac{\mu}{h_i} I + \beta D)]\underline{s}_i = -\nabla G_i + \frac{\mu}{h_i}\underline{y}_i$$

$$\underline{y}_{i+1} = \frac{\underline{s}_i}{h_i}\,, \qquad i = 0, 1, 2, \cdots \tag{4.3.15}$$

where $L_i = L(\underline{x}_i)$, $\nabla G_i = \nabla G(\underline{x}_i)$. With respect to $\underline{g}$ the iteration (4.3.14) (4.3.15) as it stands depends on "first-order information" (i.e. $J(\underline{x})$ the jacobian of $\underline{g}$) and on "second-order information" (i.e. the second derivatives of $\underline{g}$ contained in $L(\underline{x})$). Since we are interested in solving the nonlinear system (4.3.1) the need of second-order information with respect to $\underline{g}$ is a serious handicap of the methods based on (4.3.15) when compared to Newton or Quasi-Newton methods. To avoid this inconvenience, $L(\underline{x})$ in (4.3.15) has been substituted with

$$\tilde{L}\,(\underline{x}) = 2\, J^T(\underline{x})\, J(\underline{x}) \tag{4.3.16}$$

We note that the term $\sum_{i=1}^{n} g_i(\underline{x})H_i(\underline{x})$ that we have dropped in substituting $\tilde{L}$ to L is zero at the solutions $\underline{x}^*$ of (4.3.1). Iteration (4.3.15) is therefore replaced by

$$\begin{aligned} &A_i \underline{s}_i = \underline{b}_i\,, \\ &\underline{y}_{i+1} = \frac{\underline{s}_i}{h_i}\,, \qquad i = 0, 1, 2, \cdots \end{aligned} \tag{4.3.17}$$

where

$$A_i = \tilde{L}_{\,i} + \frac{1}{h_i}(\frac{\mu}{h_i} I + \beta D)\,,$$

$$\underline{b}_i = -\nabla G_i + \frac{\mu}{h_i}\underline{v}_i , \tag{4.3.18}$$

with $\tilde{L}_i = \tilde{L}(\underline{x}_i)$.

Since A_i is an $n \times n$ symmetric and positive-definite matrix the linear system in (4.3.17) can be solved by the conjugate-gradients (C.G.) method introduced by Fletcher and Reeves [15]. This procedure solves an $n \times n$ linear system in at most n steps. However, since we plan to apply the present method to large problems ($n \simeq 1000$), in order to save computational effort we solve the linear system in (4.3.17) only in an inexact way, by stopping the C.G. procedure after a number of steps which is usually considerably lower than n; this is performed by means of the following stopping criterion. Let $\underline{s}_i^{(k)}$ be the (approximate) value for the solution $\underline{s}_i$ of the linear system in (4.3.17) obtained as the result of step k of the C.G. procedure. The iteration is stopped after step m if

$$|| A_i \underline{s}_i^{(m)} - \underline{b}_i ||^2 \leq \eta_i || \underline{b}_i ||^2 \tag{4.3.19}$$

where η_i is a given relative error tolerance for the basic step (4.3.17) such that $\lim_{i \to \infty} \eta_i = 0$.

We note that if $\underline{x}_i$ is converging to a solution of (4.3.1) we have $\lim_{i \to \infty} || \underline{b}_i || = 0$. Similar ideas have been introduced for Newton method by Dembo, Eisenstat, and Steihaug [7]. Finally we observe that when $h_i \to \infty$ the step (4.3.17) degenerates into the Newton step for the nonlinear system (4.3.11), so that under suitable assumptions on $\underline{g}(\underline{x})$, h_i and η_i, local and superlinear convergence can be proved for the algorithm.

A complete mathematical analysis of this algorithm will be carried out later.

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Research Project: Numerical Optimization

Principal Investigator: Francesco Zirilli
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1. Statement of scientific work done during the reporting period

A class of algorithms derived from the ones used in the package DAFNE and based on the numerical integration of a Cauchy problem for a system of ordinary differential equations inspired by classical mechanics has been eveloped. These algorithms require the solution of an N x N linear system of equations at each step, the cost of solving this linear system when a large number of unknowns N is involved is the most important part of the computation. The linear system is solved by an iterative procedure (i.e. conjugate gradients) and only an approximate solution is computed (i.e. the conjugate gradient procedure is stopped after a number m of steps depending on the norm of the residual, $0 \leq m \leq N$). For these algorithms local convergence and Q-superlinear rate of convergence has been proved. The algorithms have been used to solve three complementarity problems derived from variational inequalities of mathematical physics very successfully. The complementarity problems considered had up to 900 variables. The results previously described are contained in section 4.

2. Research plans for the immediate future

In the immediate future we plan to pursue the following objectives:

(i) investigate how to adapt the SIGMA algorithm to work on problems involving thousands of independent variables

(ii) study the behavior of our methods on linear and nonlinear complementarity problems where existence and uniqueness of solution is not guaranteed

(iii) study the Karmarkar algorithm for linear programming as a continuation method involving the solution of a Cauchy problem for an ordinary differential equation.

3. Administrative actions

The following investigators are working on the contract:

(i) Francesco Zirilli
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During the period September 1, 1986 - December 31, 1986 Francesco Zirilli has been visiting:

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4. Appendix: "An inexact continuous method for the solution of large systems of equation and complementarity problems" by F. Aluffi-Pentini, V. Parisi, F. Zirilli.

The manuscript on this appendix has been submitted for publication on Mathematical Programming

AN INEXACT CONTINUOUS METHOD FOR THE SOLUTION OF LARGE SYSTEMS OF EQUATIONS AND COMPLEMENTARITY PROBLEMS[†]

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1. Introduction

Let $\mathbb{R}^N$ be the N-dimensional real euclidean space, let $\underline{x}=(x_1,x_2,\ldots,x_N)^T \in \mathbb{R}^N$ be a vector, and for $\underline{x},\underline{y} \in \mathbb{R}^N$ let $\langle \underline{x},\underline{y}\rangle = \sum_{i=1}^{N} x_i y_i$, $\|\underline{x}\| = \langle \underline{x},\underline{x}\rangle^{\frac{1}{2}}$ be the euclidean scalar product and norm; when necessary $\|\cdot\|$ will indicate also the matrix norm induced by the euclidean vector norm. Given $\underline{f} : \mathbb{R}^N \to \mathbb{R}^N$ we will be concerned with two classes of problems in this paper: the problem of solving the system of simultaneous nonlinear equations

$$\underline{f}(\underline{x}) = \underline{0} \tag{1.1}$$

that is: find $\underline{x}^* \in \mathbb{R}^N$ such that $\underline{f}(\underline{x}^*) = \underline{0}$, and the complementarity problem

$$\underline{x} \geq \underline{0} \tag{1.2}$$

$$\underline{f}(\underline{x}) \geq \underline{0} \tag{1.3}$$

$$\langle \underline{x},\underline{f}(\underline{x})\rangle = 0 \tag{1.4}$$

where $\underline{x} \geq \underline{0}$ means $x_i \geq 0$, $i=1,2,\ldots,N$, and similarly $\underline{f}(\underline{x}) \geq \underline{0}$ means $f_i(\underline{x}) \geq 0$, $i=1,2,\ldots,N$, $f_i(\underline{x})$ being the components of $\underline{f}$, that is: find $\underline{x}^*$ such that: $\underline{x}^* \geq \underline{0}$, $\underline{f}(\underline{x}^*) \geq \underline{0}$, $\langle \underline{x}^*,\underline{f}(\underline{x}^*)\rangle = 0$.

The importance of the problem of solving a system of simultaneous equations is well known. When $\underline{f}(\underline{x})=A\underline{x}+\underline{b}$ is an affine map the (linear) complementarity problem has been considered by Cottle and Dantzig in [1] and contains as special

cases the linear programming and the quadratic programming problem. In the case when $\underline{f}(\underline{x})$ is a possibly nonlinear function of $\underline{x}$ the (nonlinear) complementarity problem is a rather general problem and contains as special cases the Kuhn-Tucker first-order necessary conditions for the nonlinear programming problem and has been widely studied; see for example Gould and Tolle [2].

The linear and nonlinear complementarity problems have applications in such diverse areas of flow in porous media [3], image reconstruction [4], [5], game theory [6].

In this paper we will be concerned with the problem of the numerical solution of nonlinear systems of equations and complementarity problems. Usually complementarity problems are approached numerically with pivotal methods (for example the simplex method for linear programming). The pivotal methods are usually of the "step by step" improvement type, that is given a problem for which a solution is sought the standard approach is to attempt to define recursively a sequence of approximate solutions which have the basic property of making an improvement in a suitable "objective function". When the problem satisfies some convexity and/or monotonicity assumptions the pivotal methods are guaranteed to converge and if only a moderate number of independent variable is involved (up to few hundreds) their numerical performance is satisfactory.

In recent years there has been a growing interest in the use of continuous methods in nonlinear optimization; see

for example Allgover and Georg [7] for a review of simplicial methods in the computation of fixed points and the solution of nonlinear equations, and Bayer and Lagarias [8] for the interpretation of Karmarkar's linear programming algorithm as a method that follows a trajectory of a suitable system of ordinary differential equations. In particular the present authors have developed a method for solving systems of nonlinear equations based on the numerical integration of an initial-value problem for a system of ordinary differential equations inspired by classical mechanics [9], [10], [11], [12] and a method for global optimization based on the numerical integration of an initial value problem for a system of stochastic differential equations inspired by quantum mechanics [13], [14], [15]. In section 2 the algorithms introduced in [10] to solve systems of nonlinear equations are modified to allow for an "inexact" solution of the linear systems appearing in each iterations in the spirit of Dembo, Eisenstat and Steihaug [16]. These new algorithms are particularly effective for problems involving a large number of independent variables where the computational cost is dominated by the solution of the linear system at each step. Under suitable hypotheses local convergence and Q-superlinear convergence of these new "inexact" algorithm for nonlinear systems of equations is proved. In section 3 the complementarity problem is transformed into a nonlinear system of equations following Mangasarian [17] and the algorithms previously developed provide a class of locally convergent

Q-superlinear methods for the solution of complementarity problems. These methods are based on the idea of following a trajectory of a suitable system of differential equations inspired by classical mechanics and are not of the "step by step" improvement type. Finally in section 4 some numerical experience obtained with the algorithms of section 2 and 3 on some complementarity problems of mathematical physics is shown.

Some of the results of this paper have been announced in [18].

2. Some inexact algorithms for nonlinear systems of equations

Let $\underline{f}(\underline{x}) = (f_1(\underline{x}), f_2(\underline{x}), \ldots, f_N(\underline{x}))^T \in \mathbb{R}^N$, where $f_i(\underline{x})$, $i=1,2,\ldots,N$, are real-valued regular functions defined for $\underline{x} = (x_1, x_2, \ldots, x_N)^T \in \mathbb{R}^N$.

In order to solve the system of simultaneous equation

$$\underline{f}(\underline{x}) = \underline{0} \tag{2.1}$$

we define

$$F(\underline{x}) = \underline{f}^T(\underline{x})\, \underline{f}(\underline{x}) = \sum_{i=1}^{N} f_i^2(\underline{x}). \tag{2.2}$$

It is easy to see that $\underline{x}^*$ is an isolated solution of (2.1) if and only if $\underline{x}^*$ is an isolated minimizer of $F(\underline{x})$ and $F(x^*) = 0$.

In [9], [10], [11], [12] the idea has been proposed and developed of associating to the nonlinear system (2.1) the following system of second-order ordinary differential equations:

$$\mu \frac{d^2\underline{x}}{dt^2}(t) = -gD \frac{d\underline{x}}{dt}(t) - \nabla F(\underline{x}(t)) \qquad t \in [0, +\infty) \tag{2.3}$$

where D is a NxN positive symmetric matrix, μ, g are positive constants, $\nabla F(\underline{x})$ is the gradient of the function $F(\underline{x})$ with respect to $\underline{x}$. The equation (2.3) represents New-

ton's second law (mass x acceleration = force) for a particle of mass μ moving in $\mathbb{R}^N$ subject to the force $-\nabla F$ given by the potential F and to the dissipative force $-g\ D\ \frac{dx}{dt}$.

If $\underline{x}^*$ is an isolated minimizer of $F(\underline{x})$ then $\underline{x}(t) = \underline{x}^*$ $\forall t \in [0,+\infty)$ is a solution of (2.3); consider the Cauchy data:

$$\underline{x}(0) = \underline{\xi}_o \tag{2.4}$$

$$\frac{d\underline{x}}{dt}(0) = \underline{\eta}_o \tag{2.5}$$

and let $\underline{x}(t,\underline{\xi}_o,\underline{\eta}_o)$ be the solution of the Cauchy problem (2.3), (2.4), (2.5).

It can be shown that there exists a neighborhood $U \in \mathbb{R}^{2N}$ of $\begin{bmatrix}\underline{x}^* \\ \underline{0}\end{bmatrix} \in \mathbb{R}^{2N}$ such that if $\begin{bmatrix}\underline{\xi}_o \\ \underline{\eta}_o\end{bmatrix} \in U$ we have:

$$\lim_{t \to \infty} \|\underline{x}(t,\underline{\xi}_o,\underline{\eta}_o) - \underline{x}^*\| = 0. \tag{2.6}$$

Hence in order the solve the system of nonlinear simultaneous equations by integrating numerically the Cauchy problem (2.3), (2.4), (2.5), we are primarily interested in the equilibrium points reached asymptotically by the trajectories of (2.3) (hopefully solutions of (2.1)) instead than in the accuracy of the numerical scheme. So that of particular interest are numerical methods enjoying a special stability property called A-stability [10].

Let $t \in \mathbb{R}$, let $\underline{y}, \underline{\zeta}_o \in \mathbb{R}^m$ and $\underline{\phi}(t,\underline{y}) \in \mathbb{R}^m$ be a given function continuous in t and continuously differentiable with respect to $\underline{y}$, such that the initial-value problem:

$$(2.7) \qquad \frac{d\underline{y}}{dt}(t) = \underline{\phi}(t,\underline{y}) \qquad t \in (o,+\infty)$$

$$(2.8) \qquad \underline{y}(0) = \underline{\zeta}_o$$

has a solution $\underline{y}(t,\underline{\zeta}_o)$ for $t \in [0,+\infty)$.

The simplest choice of A-stable linearly implicit method to integrate numerically (2.7), (2.8) is:

$$(2.9) \qquad (I-h\Phi_n)(\underline{y}_{n+1}-\underline{y}_n) = h\underline{\phi}_n \qquad n=0,1,2,\ldots$$

$$(2.10) \qquad \underline{y}_o = \underline{\zeta}_o$$

where $\underline{y}_r$ is the numerically computed approximation of $\underline{y}(nh, \zeta_o)$, I is the identity matrix acting on $\mathbb{R}^m$, $h > 0$ is the stepsize, for $n=0,1,2,\ldots$ $t_n=nh$, $\underline{\phi}_n=\underline{\phi}(t_n,\underline{y}_n)$, $\Phi_n = \Phi(t_n,\underline{y}_n)$ where $\Phi(t,\underline{y}) = \frac{\partial \underline{\phi}}{\partial \underline{y}}$ is the jacobian of $\underline{\phi}$ with respect to $\underline{y}$. We note that when $\underline{\phi}(t,\underline{y}) = \Lambda \underline{y}$ is a linear map (2.9) reduces to the backward Euler method.

After rewriting (2.3) as a first-order system

$$(2.11) \qquad \frac{d\underline{x}}{dt} = \underline{v}$$

$$(2.12) \qquad \frac{d\underline{v}}{dt} = -\frac{g}{\mu} D\underline{v} - \frac{1}{\mu} \nabla F(\underline{x})$$

formulae (2.9), (2.10) with variable stepsize h_n, $n=0,1,\ldots$ (i.e. $t_o = 0$, $t_n = \sum_{i=0}^{n-1} h_i$, $n=1,2,\ldots$) are applied to (2.11), (2.12), (2.4), (2.5). In this case the map $\underline{\phi} : \mathbb{R}^{2N} \to \mathbb{R}^{2N}$ will be given by

$$(2.13) \qquad \underline{\phi} : \begin{bmatrix} \underline{x} \\ \underline{v} \end{bmatrix} \to \begin{bmatrix} \underline{v} \\ -\frac{g}{\mu} D\underline{v} - \frac{1}{\mu} \nabla F(\underline{x}) \end{bmatrix}$$

so that its jacobian matrix is given by

$$(2.14) \qquad \Phi(\underline{x}) = \begin{bmatrix} 0 & I \\ -\frac{1}{\mu} L(\underline{x}) & -\frac{g}{\mu} D \end{bmatrix}$$

where

$$(2.15) \qquad L(\underline{x}) = 2\left[J^T(\underline{x})J(\underline{x}) + \sum_{i=1}^{N} f_i(\underline{x})H_i(\underline{x})\right]$$

$J(\underline{x}) = \dfrac{\partial \underline{f}(\underline{x})}{\partial \underline{x}}$ is the jacobian of $\underline{f}$ with respect to $\underline{x}$ and $H_i(\underline{x})$ is the hessian of $f_i(\underline{x})$.

Let $\underline{s}_n = \underline{x}_{n+1} - \underline{x}_n$, $n=0,1,2,\ldots$; after some simple algebra (2.9) becomes:

$$(2.16) \qquad \left[L_n + \frac{1}{h_n}\left(\frac{\mu}{h_n} I + gD\right)\right] \underline{s}_n = -\nabla F_n + \frac{\mu}{h_n} \underline{v}_n$$

$$(2.17) \qquad \underline{v}_{n+1} = \frac{\underline{s}_n}{h_n} \qquad n=0,1,2,\ldots$$

$$(2.18) \qquad \underline{x}_{n+1} = \underline{x}_n + \underline{s}_n$$

where $L_h = L(\underline{x}_n)$, $\nabla F_n = \nabla F(\underline{x}_n)$. In order to avoid the computation of $H_i(\underline{x})$, $i=1,2,\ldots,N$, at each iteration and since we are looking for points $\underline{x}^*$ such that $\underline{f}(\underline{x}^*) = \underline{0}$ the term $\sum_{i=1}^{N} f_i(\underline{x})\, H_i(x)$ in (2.15) is dropped so that $L(\underline{x})$ is substituted with

$$(2.20) \qquad \tilde{L}(\underline{x}) = 2\, J^T(\underline{x}) J(\underline{x}).$$

Equation (2.16) will be replaced with

$$(2.21) \qquad A_n \underline{s}_n = \underline{b}_n$$

where

$$(2.22) \qquad A(\underline{x},h) = \tilde{L}(\underline{x}) + \frac{1}{h}\left[\frac{\mu}{h} I + gD\right]$$

and

$$(2.23) \qquad A_n = A(\underline{x}_n, h_n)$$

$$(2.24) \qquad \underline{b}_n = -\nabla F_n + \frac{\mu}{h_n} \underline{v}_n$$

we note that the matrix A_n is symmetric and positive definite.

We have the following theorem:

Theorem 2.1: Let $\underline{f} : \mathbb{R}^N \to \mathbb{R}^N$ be twice continuously differentiable, $F(\underline{x}) = \underline{f}^T(\underline{x})\, \underline{f}(\underline{x})$ and $L(\underline{x})$ be given by (2.15). Let $\underline{x}^* \in \mathbb{R}^N$ be such that $\underline{f}(\underline{x}^*) = \underline{0}$, $J(\underline{x}^*)$ is nonsingular (i.e. $\underline{x}^*$ is a nondegenerate solution of the system (2.1)) and the following Lipschitz condition holds:

$$(2.25) \qquad \|L(\underline{x}) - L(\underline{x}^*)\| \leq \gamma \|\underline{x}-\underline{x}^*\|$$

$$\forall \underline{x} \in S = \{\underline{x} \mid \|\underline{x}-\underline{x}^*\| < \sigma\}$$

for some constants γ and σ greater than zero. In the iteration (2.21), (2.17), (2.18) let $\{h_n\}$, $n=0,1,2,\ldots$, be a sequence of positive numbers such that

$$(2.26) \qquad \lim_{n \to \infty} h_n = \infty$$

then there exists $\bar{h} > 0$ such that for $h_n > \bar{h}$, $n=0,1,\ldots$, $\underline{x}^*$ is a point of attraction of (2.21), (2.17), (2.18) and the rate of convergence is

(i) Q-superlinear if $h_n^{-1} \leq \gamma_1 \|\nabla F(\underline{x}_n)\|$, $\gamma_1 > 0$, $n > n_o$, for some $\gamma_1, n_o > 0$

(ii) Q-quadratic if $h_n^{-1} \leq \gamma_2 \|\nabla F(\underline{x}_n)\|^2$, $\gamma_2 > 0$, $n \geq n_o$, for some $\gamma_2, n_o > 0$

Proof: Let us rewrite (2.21), (2.17), (2.18) as

$$\underline{x}_{n+1} = \underline{G}(\underline{x}_n, h_n) + \frac{\mu}{h_n h_{n-1}} A_n^{-1}(\underline{x}_n - \underline{x}_{n-1}) \quad n=0,1,2,... \tag{2.27}$$

where

$$\underline{G}(\underline{x},h) = \underline{x} - A(\underline{x},h)^{-1} \nabla F(\underline{x}) \tag{2.28}$$

with the initial conditions $\underline{x}_o = \underline{\xi}_o$, $\underline{x}_{-1} = \underline{\xi}_o - h_o \underline{\eta}_o$, that is (2.21), (2.17), (2.18) can be interpreted as a two-step iteration. Since $\underline{x}^*$ is a nondegenerate solution of the system (2.1) $\underline{x}^*$ is an isolated minimizer of $F(\underline{x})$ and $\nabla F(x^*) = 0$. Moreover for $h > 0$ the symmetric matrix $A(\underline{x},h)$ is positive definite so that $A(\underline{x},h)^{-1}$ exists that is $G(\underline{x},h)$ is well defined for $\underline{x} \in \mathbb{R}^N$ and $h > 0$ and $\underline{x}^*$ is a fixed point of $\underline{G}(\underline{x},h)$.

Let $\beta = \|L(\underline{x}^*)^{-1}\|$ and let $\varepsilon \in (0, \frac{1}{2}\beta^{-1})$ then there exists $\delta > 0$ and $\bar{k} > 0$ such that:

$$\|L(\underline{x}^*) - A(\underline{x},h)\| \leq \varepsilon \quad \forall \underline{x} \in S = \{\underline{x} \mid \|\underline{x}-\underline{x}^*\| \leq \delta\} \tag{2.29}$$

$$\forall h > \bar{h}$$

In fact

$$\|L(\underline{x}^*) - A(\underline{x},h)\| \leq \|L(\underline{x}^*) - \tilde{L}(\underline{x})\| + \|\tilde{L}(\underline{x}) - A(\underline{x},h)\|$$

since $L(\underline{x}^*) = \tilde{L}(\underline{x}^*)$ there exists δ such that:

$$\|L(\underline{x}^*) - \tilde{L}(\underline{x})\| \leq \tfrac{1}{2}\,\varepsilon \qquad \forall\, \underline{x} \in S$$

and for a suitable $\bar{h} > 0$

$$(2.30) \qquad \|L(\underline{x}) - A(\underline{x},h)\| = \frac{1}{h}\,\left\|\frac{\mu}{h}\,I + gD\right\| \leq \tfrac{1}{2}\,\varepsilon \qquad \forall h > \bar{h}$$

From (2.29) and the perturbation lemma (lemma 2.3.2 pag. 45 of Ortega and Rheinboldt [19]) it follows that $A(\underline{x},h)^{-1}$ satisfies

$$(2.31) \qquad \|A(\underline{x},h)^{-1}\| \leq \alpha = \frac{\beta}{1-\beta\varepsilon} \qquad \forall \underline{x} \in S,\ \forall h > \bar{h}$$

Moreover

$$(2.32) \qquad \|\underline{G}(\underline{x},h) - \underline{x}^*\| \leq \omega(\underline{x},h)\,\|\underline{x} - \underline{x}^*\| \qquad \forall \underline{x} \in S,\quad h > \bar{h}$$

where

$$(2.33) \qquad \omega(\underline{x},h) = \alpha\,[\|A(\underline{x},h) - L(\underline{x})\| + \|L(\underline{x}) - \tilde{L}(\underline{x}^*)\| + \|q(\underline{x})\|]$$

and

$$q(\underline{x}) = \begin{cases} 0 & \underline{x} = \underline{x}^* \\ \dfrac{\|\nabla F(\underline{x}) - \nabla F(\underline{x}^*) - L(x^*)(\underline{x} - \underline{x}^*)\|}{\|\underline{x} - \underline{x}^*\|} & \underline{x} \neq \underline{x}^* \end{cases}$$

In fact

$$\|\underline{G}(\underline{x},h)-\underline{x}^*\| = \|A(\underline{x},h)^{-1}[A(\underline{x},h)(\underline{x}-\underline{x}^*)-\nabla F(\underline{x})\|$$

$$\leq \alpha\{[\|A(\underline{x},h)-L(\underline{x})\|+\|L(\underline{x})-\tilde{L}(\underline{x}^*)\|]\|\underline{x}-\underline{x}^*\| +$$

$$+\|\tilde{L}(\underline{x}^*)(\underline{x}-\underline{x}^*)+\nabla F(\underline{x}^*)-\nabla F(\underline{x})\|\}.$$

Moreover from (2.25) and proposition 3.2.5 pag. 70 of [19] we have

$$(2.34) \qquad \|q(\underline{x})\| \leq \alpha_1 \|\underline{x}-\underline{x}^*\| \qquad \forall \underline{x} \in S.$$

Hence from (2.30), (2.25) and (2.34) for some constants $\alpha_2, \alpha_3 > 0$ we have

$$(2.35) \qquad \omega(\underline{x},h) \leq \alpha_2 \frac{1}{h} + \alpha_3\|\underline{x}-\underline{x}^*\| \qquad \forall \underline{x} \in S, \quad h > \bar{h}$$

From (2.27), (2.31), (2.32) for $\underline{x}_n, \underline{x}_{n-1} \in S$ and $h_n > \bar{h}$ we have

$$(2.36) \qquad \|\underline{x}_{n+1}-\underline{x}^*\| \leq \|\underline{G}(\underline{x}_n,h_n)-\underline{x}^*\| + \frac{\mu}{h_n h_{n-1}}\|A_n^{-1}[(\underline{x}_n-\underline{x}^*)+(\underline{x}^*-\underline{x}_{n-1})]\|$$

$$\leq [\omega(\underline{x}_n,h_n)+\frac{\mu\alpha}{h_n h_{n-1}}]\|\underline{x}_n-\underline{x}^*\| + \frac{\mu\alpha}{h_n h_{n-1}}\|x_{n-1}-\underline{x}^*\|)$$

$$\leq [\alpha_3\delta+\alpha_2\frac{1}{\bar{h}}+\frac{\mu\alpha}{\bar{h}^2}]\|\underline{x}_n-\underline{x}^*\| + \frac{\mu\alpha}{\bar{h}^2}\|\underline{x}_{n-1}-\underline{x}^*\|$$

Moreover from (2.35) eventually changing the values of σ and $\bar{h}$ we have

$$\gamma_3 = \alpha_3 \delta + \frac{\alpha_2}{\bar{h}} + \frac{\mu\alpha}{\bar{h}^2} < \frac{1}{2}$$

(2.37)

$$\gamma_4 = \frac{\mu\alpha}{\bar{h}^2} < \frac{1}{2}$$

so that

$$(2.38) \qquad \|\underline{x}_{n+1}-\underline{x}^*\| < \gamma_3 \|\underline{x}_n-\underline{x}^*\| + \gamma_4 \|\underline{x}_{n-1}-\underline{x}^*\|$$

with $\alpha_4 = \gamma_3 + \gamma_4 < 1$ that is $\underline{x}_{n+1} \in S$. In particular we have shown that

$$(2.39) \qquad \lim_{n\to\infty} \underline{x}_n = \underline{x}^*$$

that is $\underline{x}^*$ is a point of attraction of (2.27).

In particular for $n > n_o > 0$, $\underline{x}_n \in S$, using (2.35) the required order of convergence estimates follow from:

$$(2.40) \qquad \|\underline{x}_{n+1}-\underline{x}\| \leq [\alpha_2 \frac{1}{h_n} + \|\underline{x}_n-\underline{x}\|] \|\underline{x}_n-\underline{x}\| + \frac{\mu\alpha}{h_n h_{n-1}} \|\underline{x}_n-\underline{x}_{n-1}\|$$

for $n > n_o > 0$

and the fact that

$$(2.41) \qquad \| F(x_n) \| \leq (\| L(\underline{x}^*) \| + \varepsilon_n) \| \underline{x}_n - \underline{x}^* \|$$

where $\lim_{n \to \infty} \varepsilon_n = 0$.

Using the method given by (2.21), (2.17), (2.18) requires the solution of the linear system (2.21) at each step. Computing the exact solution with a direct method such as Gaussian elimination is very expensive when a large number of unknowns is involved and may not be worthwhile when $\underline{x}_k$ is far from $\underline{x}^*$. In this case it seems natural to solve the linear system (2.21) by an iterative procedure and to accept an approximate solution. In particular since the matrix A_n is symmetric and positive definite we may use conjugate gradients. When then method given by (2.21), (2.17), (2.18) is used solving (2.21) with an iterative procedure and accepting an approximate solution we will describe this procedure as an inexact method.

Let $\hat{\underline{s}}_n$ be the approximate step computed by the iterative procedure when solving (2.21) and

$$(2.42) \qquad \underline{r}_n = A_n \hat{\underline{s}}_n - \underline{b}_n$$

be the residual. When $\underline{r}_n = \underline{0}$ the linear system is solved exactly and $\hat{\underline{s}}_n = \underline{s}_n$. Let us assume that the approximate step computed $\hat{\underline{s}}_n$ satisfies the following condition:

$$(2.43) \qquad \|\underline{r}_n\| < \hat{\beta}_n \|\underline{b}_n\| \qquad n = 0,1,\ldots$$

for some forcing sequence $\{\hat{\beta}_n\}$, $n=0,1,\ldots$

We have the following theorem:

Theorem 2.2: Let $\underline{f}: \mathbb{R}^N \to \mathbb{R}^N$ be twice continously differentiable, $F(\underline{x}) = \underline{f}^T(\underline{x})\,\underline{f}(\underline{x})$ and $L(\underline{x})$ be given by (2.15). Let $\underline{x}^* \in \mathbb{R}^N$ be such that $\underline{f}(\underline{x}^*) = \underline{0}$, $J(\underline{x}^*)$ is nonsingular and the following Lipschitz condition holds:

$$(2.44) \qquad \|L(\underline{x})-L(\underline{x}^*)\| \leq \gamma \|\underline{x}-\underline{x}^*\| \qquad \forall \underline{x} \in S = \{\underline{x} \mid \|\underline{x}-\underline{x}^*\| < \delta\}$$

for some constants γ, δ greater than zero. In the iteration (2.21), (2.17), (2.18) let $\{h_n\}$, $n=0,1,2,\ldots$, be a sequence of positive numbers and let the linear system (2.21) be solved approximately in such a way that the residual $\underline{r}_n$ given by (2.42) satisfy the condition (2.43) for some forcing sequence $\{\hat{\beta}_n\}$, $n=0,1,\ldots$. If $0 < \hat{\beta}_n \leq \beta_{max} < 1$, $n=0,1,\ldots$, then there exists $\bar{h} > 0$ such that if $h_n > \bar{h}$, $n=0,1,\ldots$, then $\underline{x}^*$ is a point of attraction of the inexact method (2.21), (2.17), (2.18).

Proof: Since $J(\underline{x}^*)$ is nonsingular and $L(\underline{x}^*) = 2J^T(\underline{x}^*)J(x^*)$ we define the following norm:

$$(2.45) \qquad \|\underline{x}\|_* = \|L(\underline{x}^*)\underline{x}\| \qquad \forall \underline{x} \in \mathbb{R}^N$$

we have

$$(2.46)\qquad \frac{1}{\mu_1}\,\|\underline{x}\| \le \|\underline{x}\|_* \le \mu_1\|\underline{x}\| \qquad \forall \underline{x}\in \mathbb{R}^N$$

where

$$(2.47)\qquad \mu_1 = \max\{\|L(\underline{x}^*)\|, \|L(\underline{x}^*)^{-1}\|\}.$$

Moreover it is easy to see that under the stated hypothesis for any $\epsilon > 0$ there exists $\delta > 0$ and $\bar{h} > 0$ such that:

$$(2.48)\qquad \|A(\underline{x},h)-L(\underline{x}^*)\| \le \epsilon \qquad \forall \underline{x}\in S=\{\underline{x}\,|\,\|\underline{x}-\underline{x}^*\|<\delta\},\ h>\bar{h}$$

$$(2.49)\qquad \|A(\underline{x},h)^{-1}-L(\underline{x}^*)^{-1}\| \le \epsilon \qquad \forall \underline{x}\in S=\{\underline{x}\,|\,\|\underline{x}-\underline{x}^*\|<\delta\},\ h>\bar{h}$$

$$(2.50)\qquad \|\nabla F(\underline{x})-\nabla F(\underline{x}^*)-L(\underline{x}^*)(\underline{x}-\underline{x}^*)\| \le \epsilon\|\underline{x}-\underline{x}^*\| \qquad \forall \underline{x}\in S=\{\underline{x}\,|\,\|\underline{x}-\underline{x}\|^*<\delta\}$$

We have

$$(2.51)\qquad L(\underline{x}^*)(\hat{\underline{x}}_{n+1}-\underline{x}^*)=[I+L(\underline{x}^*)(A_n^{-1}-L(\underline{x}^*)^{-1})]$$

$$\cdot[\underline{r}_n+(A_n-L(\underline{x}^*))(\hat{\underline{x}}_n-\underline{x}^*)-[-\underline{b}_n-\nabla F(\underline{x}^*)-L(\underline{x}^*)(\hat{\underline{x}}_n-\underline{x}^*)]\}$$

and taking norms:

$$(2.52)\qquad \|\hat{\underline{x}}_{n+1}-\underline{x}^*\|_* \le [1+\|L(\underline{x}^*)\|\,\|A_n^{-1}-L(\underline{x}^*)^{-1}\|]$$

$$\cdot[\,\|\underline{r}_n\|+\|A_n-L(\underline{x}^*)\|\,\|\hat{\underline{x}}_n-\underline{x}^*\|+\|-\underline{b}_n-\nabla F(\underline{x}^*)-L(\underline{x}^*)(\hat{\underline{x}}_n-\underline{x}^*)\|\,]$$

from (2.24) if $\hat{x}_n \in S$ and $h_n > \bar{h}$ using (2.48), (2.49), (2.50) we have:

$$(2.53)\qquad \|\hat{x}_{n+1}-x^*\|_* \le [1+\mu_1\varepsilon][\hat{\beta}_n\|\nabla F(\hat{x}_n)\|+\varepsilon\|\hat{x}_n-x^*\|+$$

$$\varepsilon\|\hat{x}_n-x^*\|+\frac{\mu}{\bar{h}\,h_{n-1}}(1+\hat{\beta}_n)(\|\hat{x}_n-x^*\|+\|x^*-\hat{x}_{n-1}\|)]$$

moreover from

$$(2.54)\qquad \nabla F(\hat{x}_n) = L(x^*)(\hat{x}_n-x^*)+[\nabla F(\hat{x}_n)-\nabla F(x^*)-L(x^*)(\hat{x}_n-x^*)]$$

we have

$$(2.55)\qquad \|\nabla F(\hat{x}_n)\| \le \|\hat{x}_n-x^*\|_*+\varepsilon\|\hat{x}_n-x^*\|.$$

Finally from (2.47), (2.53), (2.55) we have:

$$(2.56)\qquad \|\hat{x}_{n+1}-x^*\|_* \le [1+\mu_1\varepsilon]\ [\beta_{max}(1+\varepsilon\mu_1)+\varepsilon\mu_1(2+\frac{\mu}{\bar{h}^2})]$$

$$\cdot\|\hat{x}_n-x^*\|_*+[1+\mu_1\varepsilon]\ \frac{\mu_1\mu}{\bar{h}^2}(1+\beta_{max})\|\hat{x}_{n-1}-x^*\|$$

$$= \alpha_5\|\hat{x}_n-x^*\|_*+\alpha_6\|\hat{x}_{n-1}-x^*\|$$

where

$$(2.57) \qquad \alpha_5 = [1+\mu_1\varepsilon][\beta_{max}(1+\varepsilon\mu_1)+\varepsilon\mu_1(2+\frac{\mu}{\bar{h}^2})]$$

$$\alpha_6 = (1+\mu_1\varepsilon)(1+\beta_{max})\ (\mu\mu_1/\bar{h}^2)$$

choosing the values of ε and $\bar{h}$ so that $\alpha_5+\alpha_6 < 1$ from (2.56) we have that if $\underline{\hat{x}}_n, \underline{\hat{x}}_{n-1} \in S$ then $\underline{x}_{n+1} \in S$ and

$$\lim_{n \to \infty} \underline{\hat{x}}_n = \underline{x}^*$$

Theorem 2.3: Let $\underline{f}: \mathbb{R}^N \to \mathbb{R}^N$ be twice continously differentiable, $F(\underline{x}) = \underline{f}^T(\underline{x})\ \underline{f}(\underline{x})$ and $L(\underline{x})$ be given by (2.15). Let $\underline{x}^* \in \mathbb{R}^N$ be such that $\underline{f}(\underline{x}^*) = \underline{0}$, $J(\underline{x}^*)$ is nonsingular and the following Lipschitz condition holds:

$$(2.58) \qquad \|L(\underline{x})-L(\underline{x}^*)\| \leq \gamma \|\underline{x}-\underline{x}^*\| \qquad \forall \underline{x}\ \ S=\{\underline{x} \mid \|\underline{x}-\underline{x}^*\| < \delta\}$$

In the iteration (2.21), (2.17), (2.18) let $\{h_n\}$, $n=0,1,\ldots$, be a sequence of positive numbers and let the linear system (2.21) be solved approximately in such a way that residual $\underline{r}_n$ given by (2.42) satisfy the condition (2.43) for some forcing sequence $\{\hat{\beta}_n\}$, $n=0,1,\ldots$, such that $0 < \hat{\beta}_n < \hat{\beta}_{max} < 1$, $n=0,1,\ldots$. Then there exists $\bar{h}$ such that if $h_n > \bar{h}$, $n=0,1,\ldots$, $\underline{x}^*$ is a point of attraction of the inexact method (2.21), (2.17), (2.18) and the rate of convergence is:

(i) Q-superlinear if $h_n^{-1} \leq \gamma_1 \|\nabla F(\hat{\underline{x}}_n)\|$, $\gamma_1 > 0$, $n > n_o$ for some $\gamma_1, n_o > 0$ and $\lim_{n \to \infty} \hat{\beta}_n = 0$

(ii) Q-quadratic if $h_n^{-1} \leq \gamma_2 \|\nabla F(\hat{\underline{x}}_n)\|^2$, $\gamma_2 > 0$, $n > n_o$ and $\hat{\beta}_n \leq \gamma_2 \|\nabla F(\hat{\underline{x}}_n)\|$ $n > n_o$ for some γ_2, $n_o > 0$.

Proof: From Theorem 2.2 we have that $\underline{x}^*$ is a point of attraction of the inexact method (2.21), (2.17), (2.18) so that we can assume that $\lim_{n \to \infty} \hat{\underline{x}}_n = \underline{x}^*$ and it remains to prove the rate-of-convergence results

We have:

$$(2.59) \quad \hat{\underline{x}}_{n+1} - \underline{x}^* = A_n^{-1} \{ \underline{r}_n + [A_n - L(\underline{x}^*)](\hat{\underline{x}}_n - \underline{x}^*) - [-\underline{b}_n - \nabla F(\underline{x}^*) + L(\underline{x}^*)(\hat{\underline{x}}_n - \underline{x}^*)] \}$$

and taking norms

$$(2.60) \quad \|\hat{\underline{x}}_{n+1} - \underline{x}^*\| \leq \|A_n^{-1}\| [\|\underline{r}_n\| + \|A_n - L(\underline{x}^*)\| \|\hat{\underline{x}}_n - \underline{x}^*\| + \|\nabla F(\hat{\underline{x}}_n) - \nabla F(\underline{x}^*) - L(\underline{x}^*)(\hat{\underline{x}}_n - \underline{x}^*)\| + \frac{\mu}{h_n h_{n-1}} \|\underline{x}_n - \underline{x}_{n-1}\|]$$

Let $\epsilon, \delta, \bar{h}$ be chosen in such a way that (2.29), (2.34), (2.35) hold then there exists n_o' such that for $n > n_o' + 1$, $\hat{\underline{x}}_n \in S = \{\underline{x} | \|\underline{x} - \underline{x}^*\| < \delta\}$ we have:

$$(2.61) \quad \|\hat{\underline{x}}_{n+1} - \underline{x}^*\| \leq \alpha [\hat{\beta}_n \|\nabla F(\hat{\underline{x}}_n)\| + (\alpha_2 \frac{1}{2h_n} + \alpha_3 \|\hat{\underline{x}}_n - \underline{x}^*\|) \|\hat{\underline{x}}_n - \underline{x}^*\| + \alpha_1 \|\hat{\underline{x}}_n - \underline{x}^*\|^2 + \frac{\mu}{\bar{h} h_n} (1 + \hat{\beta}_n) \|\hat{\underline{x}}_n - \hat{\underline{x}}_{n-1}\|]$$

and the desired rate-of-convergence results follow from (2.41).

3. Complementarity problems and nonlinear systems

Let $\underline{f}: \mathbb{R}^N \to \mathbb{R}^N$ be given, the complementarity problem associate with $\underline{f}$ is

$$\underline{x} \geq \underline{0} \tag{3.1}$$

$$\underline{f}(\underline{x}) \geq \underline{0} \tag{3.2}$$

$$\langle \underline{x}, \underline{f}(\underline{x}) \rangle = 0 \tag{3.3}$$

and let $\theta: \mathbb{R} \to \mathbb{R}$ be a strictly increasing function such that $\theta(0) = 0$. In [17] Mangasarian has shown that $\underline{x}^* \in \mathbb{R}^N$ is a solution of the complementarity problem (3.1), (3.2), (3.3) if and only if $\underline{x}^*$ is a solution of the system of nonlinear equations

$$\underline{g}(\underline{x}) = \underline{0} \tag{3.4}$$

where $\underline{g}(\underline{x}) = (g_1(\underline{x}), g_2(\underline{x}), \ldots, g_N(\underline{x}))^T$ and

$$g_i(\underline{x}) = \theta(|f_i(\underline{x}) - x_i|) - \theta(f_i(\underline{x})) - \theta(x_i) \tag{3.5}$$

$$i = 1, 2, \ldots, N$$

for later purposes let us introduce

$$G(\underline{x}) = \underline{g}(\underline{x})^T \underline{g}(\underline{x}) \tag{3.6}$$

Definition 3.1: Let $\underline{x}^* \in \mathbb{R}^N$ be a solution of the complementarity problem (3.1), (3.2), (3.3) we will say that $\underline{x}^*$ is nondegenerate if $\underline{x}^* + \underline{f}(\underline{x}^*) > \underline{0}$.

Definition 3.2: Let $\underline{f}$ be continuously differentiable and $J(\underline{x}) = \frac{\partial \underline{f}}{\partial \underline{x}}$ be the jacobian of $\underline{f}$ with respect to $\underline{x}$, if for $\bar{n} = 1,2,\ldots,N$ the principal minor $((\frac{\partial f_i}{\partial x_j}))$, $i,j=1,2,\ldots,\bar{n}$, is nonsingular we say that $(J(\underline{x})$ has nonsingular principal minors.

In [17] Mangasarian has shown that if $\underline{x}^*$ is a nondegenerate solution of the complementarity problem (3.1), (3.2), (3.3) such that $J(\underline{x}^*)$ has nonsingular principal minors and θ: $\mathbb{R} \to \mathbb{R}$ is a stricty increasing differentiable function such that $\frac{d\theta}{dt}(0) + \frac{d\theta}{dt}(t) > 0 \quad \forall t > 0$ then $\underline{x}^*$ is a solution of the nonlinear system (3.4) and $\frac{\partial \underline{g}}{\partial \underline{x}}(\underline{x}^*)$ the jacobian of $\underline{g}$ with respect $\underline{x}$ is nonsingular.

For simplicity we choose $\theta(t) = \frac{t}{2}$ so that in a neighborhood of a nondegenerate solution of the complementarity problem (3.1), (3.2), (3.3) the function $\underline{g}(\underline{x})$ given by (3.5) has the same regularity properties of $\underline{f}(\underline{x})$. Given the local character of the convergence theorems of section 2 this is satisfactory. In section 4 the method for solving nonlinear system described in section 2 will be applied to (3.4) with $\theta(t) = \frac{t}{2}$ for some test complementarity problems.

4. Numerical experience

The inexact method (2.21), (2.17), (2.18) has been implemented as follows:

(i) since A_n is symmetric and positive definite the linear system (2.21) has been solved by the conjugate gradient method (C.G.) introduced by Fletcher and Reeves [20]. This procedure solves an N x N linear system in at most N steps. Hovewer we stop the conjugate gradient procedure after a number of steps which is usually considerably lower than N. In fact let $\underline{s}_n^{(k)}$ be the approximate value for the solution $\underline{s}_n$ of the linear system (2.21) obtained as the result of step k of the conjugate gradient procedure. The conjugate gradient iteration is stopped after step m if

$$\| A_n \underline{s}_n^{(m)} - \underline{b}_n \| \leq \hat{\beta}_n \| b_n \|$$

ii) we have chosen:

$$\underline{\xi}_o = \underline{\eta}_o = \underline{0}$$

$$\mu = g = 1$$

$$D = I \text{ (the identy matrix)}$$

$$\underline{s}_n^{(o)} = \underline{0} \quad n=0,1,\ldots$$

and the following very simple variation laws for the

time integration step-length h_n and the forcing sequence $\hat{\beta}_n$:

$$h_{n+1} = \min (10h_n, h_{max}) \qquad n=0,1,2,...$$

with $h_o=1$, $h_{max} = 10^{35}$

$$\hat{\beta}^2_{n+1} = \hat{\alpha}_n \hat{\beta}^2_n \qquad n=0,1,2,...$$

where $\hat{\beta}_o$ is given and $\hat{\alpha}_n$ is automatically chosen by the program among the two values 0.1 and 0.5.

iii) the program stops in any case the conjugate-gradients iteration after N steps in order to avoid possible non termination due to the finite arithmetic of the computer.

Finally the method given by (2.21), (2.17), (2.18) (i.e. exact solution of the linear system (2.21)) is obtained simply setting $\hat{\beta}_o = 0$.

The stopping rule adopted is $G(\underline{\hat{x}}_n) \leq 10^{-10}$ for the inexact method and $G(\underline{x}_n) \leq 10^{-10}$ for the "exact" method (i.e. $\hat{\beta}_o = 0$). These methods have been coded in the Pascal programming language and the program has been run on a Hewlett-Packard 9816 computer.

We have tested the proposed algorithm on three complementarity problems of which two are linear and one is nonlinear.

The first problem considered arises as a one-dimensio-

nal free-boundary problem in the lubrication theory of an infinite journal bearing, i.e. a rotating cylinder separated from a bearing surface by a thin film of lubricating fluid [21]. The finite-difference approximation used by Cryer in [21] leads to

Problem A (called Problem 3D by Cryer): Find $\underline{x}$, $\underline{w} \in \mathbb{R}^N$ such that

$$(4.1) \qquad \underline{w} = \underline{q} + M\underline{x}, \quad \underline{w} \geq \underline{0}, \quad \underline{x} \geq \underline{0},$$

$$(4.2) \qquad < \underline{w}, \underline{x} > = 0,$$

where $M = ((M_{ij}))$, $i,j=1,2,\ldots,N$ is an N x N matrix with elements M_{ij} given by

$$(4.3) \qquad \begin{aligned} M_{ij} &= -(H_{i+\frac{1}{2}})^3, && \text{if } j = i+1, \\ M_{ij} &= [(H_{i+\frac{1}{2}})^3 + (H_{i-\frac{1}{2}})^3], && \text{if } j = i, \\ M_{ij} &= -(H_{i-\frac{1}{2}})^3, && \text{if } j = i-1, \\ M_{ij} &= 0, && \text{otherwise} \end{aligned}$$

and $\underline{q} = (q_1, q_2, \ldots, q_N)^T$ is a vector with elements q_i given by

$$(4.4) \qquad q_i = \frac{T}{N+1} [H_{i+\frac{1}{2}} - H_{i-\frac{1}{2}}], \qquad i=1,2,\ldots N$$

where

$$H_{i\pm\frac{1}{2}} = H((i\pm\tfrac{1}{2})\frac{T}{N+1} \tag{4.5}$$

and the function H(y) is given by

$$H(y) = \frac{1}{\sqrt{\pi}}(1+\varepsilon\cos\pi y) > 0 \tag{4.6}$$

with

$$T = 2, \quad \varepsilon = 0.8 \tag{4.7}$$

We note that the matrix M given by (4.3) is symmetric and positive-definite.

The second problem arises as a two-dimensional free-boundary problem in the theory of the steady-state fluid flow through porous media. Some of these problems can be formulated as a variational inequality after an ingenious transformation proposed by Baiocchi and others (ref. [3]). The discretization used on the "model problem" ([3], p. 4) leads to

Problem B: Find $\underline{x}$, $\underline{w} \in \mathbb{R}^N$ such that

$$\underline{w} = \underline{q} + M\underline{x}, \quad \underline{w} \geq 0, \quad \underline{x} \geq 0, \tag{4.8}$$

$$\langle \underline{w}, \underline{x} \rangle = 0 \tag{4.9}$$

where M, an N x N real matrix, and $\underline{q} = (q_1, q_2, \ldots, q_N)^T \in \mathbb{R}^N$ are defined below.

Given n_x, n_y (positive integers) and X, Y (positive real numbers), let

$$N = n_x n_y,$$

$$Dx = X/(n_x+1),$$

$$Dy = Y/(n_y+1)$$

$$a = Dy/Dx,$$

let A be the n_x x n_x tridiagonal matrix having all the main diagonal elements equal to $2(a+1/a)$, and the paradiagonal elements (i.e. immediately above or below the main diagonal) equal to -a, and let B be the n_x x n_x diagonal matrix with diagonal elements equal to -1/a. The matrix M is an n x n matrix with a block-tridiagonal structure (n_y x n_y blocks), having each main-diagonal block equal to the matrix A, and each paradiagonal block equal to the matrix B. We note that M is a positive-definite symmetric matrix. The vector $\underline{q}$ is defined as follows. Given $W(0 < W < Y)$, and using the Kronecker symbol δ_{ij}, let

$$g_L(y) = \tfrac{1}{2}(Y-y)^2,$$

$$g_R(y) = \tfrac{1}{2}(W-y)^2, \qquad \text{if } y < W,$$

$$g_R(y) = 0, \qquad \text{if } y \geq W,$$

$$g_D(x) = Y^2/2-(Y^2-W^2)(x/2X),$$

$$g_U(x) = 0,$$

$$r_{ij} = -Dx\ Dy + \delta_{i1}\ a\ g_L(j\ Dy)+\delta_{in_x}\ a\ g_R(j\ Dy)$$

$$+ \delta_{ij}(1/a)g_D(i\ Dx) + \delta_{n_y j}(1/a)g_U(i\ Dx),$$

$$i = 1,2,\ldots,n_x, \qquad j = 1,2,\ldots,n_y.$$

The elements $q_1,q_2,\ldots,q_n$ of $\underline{q}$ are given by

$$(4.10) \qquad q_k = r_{ij}, \quad \text{with} \quad k = (j-1)n_x+i$$

Our last problem, which is defined below, can be interpreted as a finite-difference approximation of a nonlinear variational inequality.

Problem C: Find $\underline{x}$, $\underline{w} \in \mathbb{R}^N$ such that

$$(4.15) \qquad \underline{w} = M\underline{x} + \underline{p}(\underline{x}) + \underline{q}, \qquad \underline{w} \geq 0, \quad \underline{x} \geq 0$$

$$(4.16) \qquad \langle \underline{w},\underline{x} \rangle = 0$$

The problem dimension N, the quantities Dx, Dy and the matrix M are defined as in problem B, given n_x,n_y,X,Y. The nonlinear term $\underline{p}(\underline{x})$ is a vector in $\mathbb{R}^N$ with components $p_i=x_i^3$, $i=1,\ldots,N$. The vector $\underline{q}=(q_1,q_2,\ldots,q_N)^T$ is defined by equation (4.10) where r_{ij} = Dx Dy sin $(2\pi\ iDx/X)$, $i=1,2,\ldots,n_x$, $j=1,2,\ldots,n_y$.

The numerical results obtained with the previously described methods on Problem A, B, C are shown in Tables 1, 2, 3 respectively.

TABLE 1 - Results of Problem A

	$\eta_o = 1$		$\eta_o = 0$	
	n. of steps (2.21)	total n. of C.G. steps	n. of steps (2.21)	total n. of C.G. steps
30	10	79	7	210
40	12	121	8	320
50	16	238	8	400
60	14	240	8	480
70	15	318	9	630
80	15	369	9	720
90	19	650	9	810
100	18	556	10	1000

TABLE 2 - Results of Problem B

(with X = 1.62, Y = 3.22, W = 0.84)

n_x	n_y	N	$\eta_o = 1$		$\eta_o = 0$	
			n. of steps (2.21)	total n. of C.G. steps	n. of steps (2.21)	total n. of C.G. steps
6	9	54	13	170	6	324
8	12	96	15	250	8	768
10	15	150	17	483	10	1500
12	18	216	19	746	12	2592
14	21	294	19	867	14	4116
20	30	600	34	2405	21	12600

TABLE 3 - Results of Problem C

(with H = 5, Y = 5)

n_x	n_y	N	$\eta_o = 1$		$\eta_o = 0$	
			n. of steps (2.21)	total n. of C.G. steps	n. of steps (2.21)	total n. of C.G. steps
5	5	25	5	37	4	100
10	10	100	6	99	5	500
15	15	225	8	278	6	1350
20	20	400	10	407	6	2400
25	25	625	10	535	8	5000
30	30	900	10	893		

In tables 1, 2, 3 the advantage of using "inexact linear algebra" with respect to complete solution of the linear system for problems A, B, C is shown, and the advantage is increasing with the number of unknowns.

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Numerical Optimization
Complementarity Problems

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20. (continued)

1. - Statement of scientific work done during the reporting period

2. - Research plans for the immediate future

3. - Administrative actions

Research Project: Numerical Optimization

Principal Investigator: Francesco Zirilli
Contractor: Università di Roma "La Sapienza"
Contract Number: DAJA45-86-C-0028
Third Periodic Report
Jan. 1987-Jul. 1987

The research reported in this document has been made possible through the support and sponsorship of the U.S. Government through its European Research Office of the U.S. Army.

I N D E X

1.- Statement of scientific work done during the reporting period

We worked on the idea of attempting to adapt the SIGMA algorithm to work on complementarity problems with many independent variables. In particular we try to exploit the following special features of the complementarity problem:

(i) the objective function is a piecewise quadratic

(ii) the objective function value to be found is zero.

The modified version of the SIGMA algorithm is much more efficient on complementarity problems than the original one. However it is unable to solve complementarity problems coming from mathematical physics such as the ones described in the First Periodic Report with more than fifty or sixty variables.

Further work is necessary.

2.- Research plans for the immediate future

In the immediate future we plan to pursue the following objectives:

(i) study the behaviour of our methods on linear and nonlinear complementarity problems where existence and uniqueness of solution is not guaranteed

(ii) study the Karmarkar algorithm for linear programming as a continuation method involving the solution of a Cauchy problem for an ordinary differential equation.

3.- Administrative actions

The following investigators are working on the contract:

Francesco Zirilli
Dipartimento di Matematica "G. Castelnuovo"
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Filippo Aluffi-Pentini
Dipartimento di Metodi e Modelli
Matematici per le Scienze Applicate
Università di Roma "La Sapienza"
00185 ROMA (Italy)

Valerio Parisi
Dipartimento di Fisica
II Università di Roma (Tor Vergata)
00173 ROMA (Italy)

In May 1987 Francesco Zirilli has presented an invited talk: "Some physical ideas leading to global optimization algorithms" to the SIAM Conference on Optimization held in Houston (USA), May 18-20, 1987.

After a final revision the two papers describing the SIGMA package have been accepted for publication on ACM Transactions on Mathematical Software.

Research Project: Numerical Optimization

Principal Investigator: Francesco Zirilli

Contractor: Università di Roma "La Sapienza"

Contract Number: DAJA 45-86-C-0028

Fourth Periodic Report

Jul 87 - Jan 88

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Numerical Optimization
Complementarity Problems

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

This is the Fourth Periodic Report on Contract DAJA 45-86-C-0028; it contains
(1) Statement of scientific work done during the reporting period
(2) Research plans for the immediate future
(3) Administrative actions
(4) Appendix: F. Aluffi-Pentini, V. Parisi, F. Zirilli, "A parallel global optimization algorithm inspired by quantum physics," to appear in Calcolo.

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Index

§1. Statement of scientific work during the reporting period.

The solution of complementarity problems in many variables is a difficult computational problem. In order to solve complementarity problems we have pursued two goals:

(i) construct efficient numerical algorithms

(ii) exploit the new computer architectures and in particular the parallel machines.

The linear complementarity problem can be written as follows:

Problem 1. Given $A \in \mathbb{R}^{n \times n}$ and $\underline{b} \in \mathbb{R}^n$ find $\underline{x} \in \mathbb{R}^n$ such that

$$\underline{x} \geq \underline{0}$$
$$\underline{f}(\underline{x}) \equiv A\underline{x} + \underline{b} \geq 0$$
$$\langle \underline{x}, \underline{f}(\underline{x}) \rangle = 0$$

Let us define the function $F: \mathbb{R}^n \to \mathbb{R}$:

$$F(\underline{x}) = \sum_{i=1}^{n} F_i(\underline{x})$$

where

$$F_i(\underline{x}) = x_i^2 \quad \text{if} \quad x_i \geq 0, \; x_i < f_i(x)$$
$$= x_i^2 + f_i^2 \quad \text{if} \quad x_i < 0, \; f_i < 0$$
$$= f_i^2 \quad \text{if} \quad f_i \leq x_i, \; f_i \geq 0$$

It is easy to see that $F(\underline{x}) \geq 0$ and that $F(x) = 0$ if and only if $\underline{x}$ is a solution of the linear complementarity problem (Problem 1). Problem 1 is equivalent to the following global optimization problem:

Problem 2. Find the global minimizer of F, verify that the function value at the global minimizers of F is zero.

We remark that when the linear complementarity problem has many solutions the function F will have many global minimizers with zero function value, when the linear complementarity problem has no solutions the global minimizers of F will correspond to a positive function value.

In order to solve Problem 2 we have considered two algorithms:

(1) CSIGMA. A modified version of the SIGMA algorithm that makes use of a conjugate gradient technique in the time integration step. This algorithm is stochastic in nature and is explicitely designed for the search of global minimizers. The initial guess used is $\underline{x}_o = \underline{0}$

(2) GRACON. A conjugate gradient minimization technique applied to the function F from the initial guess $\underline{x}_o = \underline{0}$.

The algorithms CSIGMA and GRACON have been tested on three test problems:

Test Problem 1 is the linear complementarity problem in lubrication theory proposed by Cryer and described in detail in the First Periodic Report.

Test Problem 2: Let B be a random matrix with gaussian elements of mean zero and variance one and let $A = B^T B$. The matrix A is positive definite (to be precise A could have zero as an eigenvalue with pro

bability zero) so that the corresponding linear complementarity problem has a unique solution for any $\underline{b}$.

Test Problem 3: Let B be as in Test Problem 2 and let A = B. Since A = B is indefinite in general the corresponding linear complementarity problem may have many solutions or no solution. We choose $\underline{b}$ such that the linear complementarity problem has at least one solution. Moreover we know this solution.

The results obtained with CSIGMA and GRACON are shown in Table 1 and Table 2.

Table 1 CSIGMA

N	Test PROBL 1		Test PROBL 2		Test PROBL 3	
	ISUC	NFEV	ISUC	NFEV	ISUC	NFEV
2	1	11.772	1	8.459	2	18.673
4	1	10.361	1	48.504	2	39.141
8	1	34.826	1	44.795	2	58.175
16	1	68.717	1	51.849	2	86.336
32	1	130.851	1	87.298	2	2.829.481
64	1	156.815	1	330.777	-1	
100	1	659.009				

N	Test PROBL 1		Test PROBL 2		Test PROBL 3	
	ISUC	NFEV	ISUC	NFEV	ISUC	NFEV
2	1	15	1	25	2	2
4	1	36	1	88	1	65
8	1	77	1	109	1	122
16	1	240	1	198	2	384
32	1	708	1	627	0	479
64	1	3.158	1	1.066	0	635
100	1	7.765	1	1.523	0	1.092

Legenda

N = number of independent variables

ISUC = - 1 maximum allowed time has been exceeded

0 failure

1 success. The solution known a priori has been found

2 success. A solution different from the one known a priori has been found.

NFEV = number of function evaluations.

From Table 1 and Table 2 we can see that CSIGMA appears to be robust but not very efficient while GRACON appears to be efficient but not very robust.

Further research is pursued now to build an efficient and robust algorithm that combines the stochastic character of CSIGMA (robustness) with the local properties of GRACON (efficiency).

The second goal, that is the possibility of using a SIGMA algorithm on a parallel machine, has been studied (see §4 Appendix).

§2. Research plans for the immediate future.

In the immediate future we plan to pursue the following objectives:

(i) go back to linear and nonlinear complementarity problems that come from physical problems in order to try to find some more efficient algorithm

(ii) study the special case of linear programming in the context of continuation methods.

§3. Administrative actions.

In September 1987 Francesco Zirilli has presented the invited talk: "A parallel algorithm for global optimization inspired by quantum physics" to the conference "Vector and parallel processors for scientific computation 2" sponsored by the Accademia Nazionale dei Lincei and the IBM Italia in Rome.

The paper:

(1) F. Aluffi-Pentini, V. Parisi, F. Zirilli: "Test problems for global optimization" has been accepted for publication in The Computer Journal.

(2) F. Aluffi-Pentini, V. Parisi, F. Zirilli: "A parallel global optimization algorithm inspired by quantum physics" has been accepted for publication in Calcolo.

§4. Appendix: F. Aluffi-Pentini, V. Parisi, F. Zirilli: "A parallel global optimization algorithm inspired by quantum physics," to appear in Calcolo.

A parallel global optimization algorithm inspired by quantum physics†‡

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§1. Introduction

Let $\mathbb{R}^N$ be the N-dimensional real euclidean space, and let $\underline{x} = (x_1, x_2, \ldots, x_N)^T \in \mathbb{R}^N$, the superscript T meaning transpose, for $\underline{x}, \underline{y} \in \mathbb{R}^N$ $\langle \underline{x}, \underline{y} \rangle = \sum_{i=1}^{N} x_i y_i$ is the scalar product between $\underline{x}$ and $\underline{y}$, and $\| \underline{x} \| = \langle \underline{x}, \underline{x} \rangle^{\frac{1}{2}}$ is the euclidean norm of $\underline{x}$.

In this paper we will consider two problems, that is:

(i) Problem 1. Solving systems of equations. Let $\underline{f} = \mathbb{R}^N \to \mathbb{R}^N$ be a given map, solve the system of equations

$$\underline{f}(\underline{x}) = \underline{0} \tag{1.1}$$

that is find the points $\underline{x}^* \in \mathbb{R}^N$ such that

$$\underline{f}(\underline{x}^*) = \underline{0}$$

(ii) Problem 2. Global optimization. Let $g : \mathbb{R}^N \to \mathbb{R}$ be a given function, find the points $\underline{x}^* \in \mathbb{R}^N$ such that

$$g(\underline{x}^*) \leq g(\underline{x}) \qquad \forall\, \underline{x} \in \mathbb{R}^N \tag{1.2}$$

It is easy to see that Problem 1 can be reduced to Problem 2, in fact, $\underline{x}$ is a solution of $\underline{f}(\underline{x}) = \underline{0}$ if and only if $g(\underline{x}) = \| \underline{f}(\underline{x}) \|^2 = 0$ that is $\underline{x}$ is a global minimizer of g. Moreover, isolated solutions of the system of equations become non-degenerate minimizers of g. When Problem 1 is reduced to Problem 2 is known a priori that the minimizers of g we are interested in correspond to function value g = 0. This feature is of great value since it gives us the possibility of recognizing a global minimizer from the function value in a point.

In recent years several stochastic algorithms have been proposed to solve the global optimization problem. We remember the simulated annealing method of Kirkpatrick, Gelatt and Vecchi [1] and the bayesan approach of Rinnooy Kan and coworkers [2] while we have been advocating a method inspired by statistical and quantum mechanics [3]. Let us remember briefly the method proposed in [3]; let us consider the Cauchy problem

$$(1.3) \qquad d\underline{\xi} = -\nabla g(\underline{\xi}) + \varepsilon(t)\, d\underline{w}$$

$$(1.4) \qquad \underline{\xi}(0) = \underline{x}_0$$

where $\underline{w}(t)$ is a standard n-dimensional Wiener process $g(\underline{x})$ is the function whose global minimizers we are interested in that we assume twice continuously differentiable with only a finite number of global minimizers and such that:

$$(1.5) \qquad \lim_{\|x\| \to \infty} g(\underline{x}) = \infty$$

$$(1.6) \qquad \int_{\mathbb{R}^n} \exp(-\alpha^2 g)\, dx < \infty \qquad \forall\, \alpha \in \mathbb{R}\setminus\{0\}$$

Finally, $\varepsilon(t)$ is a continuous function such that

$$(1.7) \qquad \lim_{t \to \infty} \varepsilon(t) = 0$$

When $\varepsilon(t) = \varepsilon_0$ is a constant, equation (1.3) is known as the Smoluchowski-Kramers equation [4]. This equation is a singular limit of the Langevin equation when the inertial terms are neglected. The Smoluchowski-Kramers equation has been used widely by solid state physicists and chemists to study physical phenomena such as atomic migration in crystals or chemical reactions. In these applications $\varepsilon_0 = (2K\hat{T}/m)^{1/2}$ where $\hat{T}$ is

the absolute temperature, K the Boltzmann constant, m the reduced mass of the electron and $g(\underline{x})$ the potential energy, so that (1.3) represents diffusion across potential barriers under the stochastic forces $\varepsilon_0 d\underline{w}$. Choosing $\varepsilon = \varepsilon(t)$ with $\lim_{t\to\infty} \varepsilon(t) = 0$ corresponds to freezing the system that is $\hat{T} \to 0$.

In order to compute the global minimizers of g in [3] we have proposed to numerically integrate the trajectories of (1.3), (1.4). In fact, if $\varepsilon(t)$ goes to zero sufficiently slowly (adiabatic freezing) the stochastic process $\underline{\xi}(t)$ solution of (1.3), (1.4) will converge in law to a random variable concentrated at the global minimizers of g. In section 2 we discuss briefly the numerical aspects of this method for global optimization and in section 3 we present the advantages of a parallel version of this method.

§2. The numerical integration

In [5], [6] an implementation in a FORTRAN program of the method introduced in [3] has been realized for serial machines. A numerical method to obtain the global minimizers of g consists in a numerical integration procedure for the Cauchy problem (1.3), (1.4). The efficiency of the numerical method for global optimization obtained depends on the numerical integration scheme chosen, so that is essential to make a judicious choice. In making this choice we should consider two facts:

(i) to the purpose of obtaining global minimizers of g only asymptotic values of the trajectories are relevant so that highly accurate schemes are unnecessary.

(ii) in order to give a chance to the random forces to take the trajectory out of local minimizers many time integration steps should be computed so that only methods with a very cheap step can be considered.

With this in mind in [5], [6] we have chosen the explicit Euler method with steplength control to guarantee stability. That is, $\underline{\xi}_K$ approximation of $\underline{\xi}(t_K)$ solves the following difference equation:

$$\underline{\xi}_K - \underline{\xi}_{K-1} = -h_{K-1}\nabla g(\underline{\xi}_{K-1}) + \varepsilon(t_{K-1})(\underline{w}_K - \underline{w}_{K-1}) \qquad k = 1,2, \ldots \tag{2.1}$$

$$\underline{\xi}_0 = \underline{x}_0 \tag{2.2}$$

where $t_0 = 0$ $t_K = \sum_{i=0}^{K-1} h_i$, $h_K > 0$ and $\underline{w}_K = \underline{w}(t_K)$ $K = 0,1,2, \ldots$. To avoid the degredation of the numerical algorithm when g is ill conditioned the algorithm implemented in [5], [6] provides some form of automatic rescaling. Since in the right hand side of (2.1) there is the sum of a

deterministic term $h_{K-1}\,\nabla g(\underline{\xi}_{K-1})$ with a stochastic term $\varepsilon(t_{K-1})(\underline{w}_K - \underline{w}_{K-1})$ when they are of the same order of magnitude the effort necessary to compute accurately ∇g (N+1 function evaluations if forward finite differences are used) can be wasted adding $\varepsilon(t_{K-1})(\underline{w}_K - \underline{w}_{K-1})$. Therefore we replace the gradient ∇g with a "random gradient" as follows: let $\underline{r}$ be an N-dimensional random vector of length one uniformly distributed on the N-dimensional unit sphere. Then for any given (non-random) vector $\underline{v} \in \mathbb{R}^N$ its projection along $\underline{r}$ is such that

$$(2.3) \qquad N\,E\,(\,\langle \underline{r},\underline{v}\rangle\,\underline{r}) = \underline{v}$$

where $E(\cdot)$ is the expected value. This suggests to replace the gradient $\nabla g(\underline{\xi}_K)$ with the "random gradient":

$$(2.4) \qquad \underline{\gamma}(\underline{\xi}_K) = N\,\langle r, \nabla g(\underline{\xi}_K)\rangle\,\underline{r}$$

we note that only 2 function evaluations (*independently of* N) are necessary to evaluate $\underline{\gamma}(\underline{\xi}_K)$ with forward finite differences. Finally, due to its stochastic nature the initial value problem (1.3), (1.4) has an infinite number of trajectories even when the initial condition (1.4) is fixed. Since we are looking for trajectories that diffuse through local minimizers it is natural to compute several trajectories of (1.3), (1.4) simultaneously and independently (7 trajectories in the actual implementation of [5], [6] on a serial machine) and compare them at the end of some suitable "observation period" to choose which trajectory is worthwhile to continue to compute and which one should be abandoned on the basis of some heuristic criterion. This last feature of our algorithm makes him a natural candidate for parallelization since when more than one processor is available independent trajectories can be computed very efficiently on different processors.

§3. The parallel algorithm

In the IBM ECSEC Center in Rome a numerical experimentation on a parallel version of the algorithm for global minimization described in section 2 has been made. Since the heaviest part of the computation, that is the integration of several trajectories of the stochastic initial value problem (1.3), (1.4), can be done independently and simultaneously by several processors. The parallel version of the algorithm will have a very high speed-up factor. The numerical experimentation has been carried out on the 37 test problems presented in [7] and used to test the serial algorithm in [5], these problems include the Dixon-Szego functions and the Levy-Montalvo functions.

In the following table 1 for each one of the 37 problems are reported the following times (in msec) measured by a library routine:

T = execution time of the algorithm executed serially (only one processor active)

T1 = execution time of the processor 1 that we use as master processor so that T1 is the execution time of the algorithm executed in its parallel version (7 processors active, 7 trajectories computed)

T2,T3, ... , T7 execution time on the processor 2,3, ... , 7 respectively. Each processor computes one of the 7 trajectories. Processor 1 besides being the master computes one trajectory.

Finally, the table for each of the 37 problems reports the following quantities:

$S1 = T1 + T2 + \ldots + T7$

$S2 = T2 + T3 + \ldots + T7$

$\frac{S2}{6}$ = average execution time for a parallel processor

$\frac{T}{T1}$ = speed up time. With 7 processors we have $\frac{T}{T1} \leq 7$.

The table reports also the total on all the 37 problems of the previously described quantities. It can be observed that some data are inconsistent (for example $T1 < T2$) but this is due to experimental errors in the measurement. The total speed-up factor is 6.36, that is 91% of the maximum speed-up factor attainable 7. As expected the algorithm is very well suitable for parallelization.

Acknowledgement: One of us (F.Z.) gratefully ackhowledges the hospitality of Rice University where part of this work was done.

Table 1

Probl.	T	T1	T2	T3	T4	T5	T6	T7	S1	S2	S2/6	T/T1	S1/T
1	29320	6296	5689	5540	4940	5260	5331	5504	38560	32264	5377.33	4.66	1.315
2	19942	4864	3276	3562	3652	3499	3238	3558	25649	20785	3464.17	4.10	1.286
3	60619	11314	10182	10432	10001	10057	10189	10116	72291	60977	10162.83	5.36	1.193
4	28422	5790	5036	4813	5014	4879	4928	4839	35299	29509	4918.17	4.91	1.242
5	115435	21728	19483	19356	19474	21288	18166	21451	140946	119218	19869.67	5.31	1.221
6	37321	7365	6750	6346	6267	6791	6487	6296	46302	38937	6489.50	5.07	1.241
7	176769	27954	28360	28495	28247	27205	28029	28581	196871	168917	28152.83	6.32	1.114
8	443737	71475	70124	69374	70553	69017	70431	69311	490285	419810	69801.67	6.21	1.105
9	417124	69950	65551	64723	65427	64252	66438	65648	461989	392039	65333.83	5.96	1.108
10	26404	4963	4410	4650	4690	4442	4607	4483	32245	27282	4547.00	5.32	1.221
11	32801	6495	5591	5847	5478	5651	5753	5613	40428	33933	5655.50	5.05	1.233
12	40196	7779	6994	6937	6828	7009	6632	6886	49065	41286	6881.00	5.17	1.221
13	25020	4837	4297	4228	4329	4141	4225	4501	30558	25721	4286.83	5.17	1.221
14	23573	4767	4009	4345	3889	3940	4044	4275	29269	24502	4083.67	4.95	1.242
15	28960	5929	5207	5082	4692	4895	5124	5017	35946	30017	5002.83	4.88	1.241
16	43292	8274	7375	7512	7158	7486	7385	7837	53027	44753	7458.83	5.23	1.225
17	33643	6737	6114	5878	5888	5451	5580	5687	41335	34598	5766.33	4.99	1.229
18	331615	48860	49551	51520	51763	50694	49094	49777	351259	302399	50399.83	6.79	1.059
19	525142	76481	81909	78854	78239	77179	80829	78673	552164	475683	79280.50	6.87	1.051
20	494787	76326	74264	72637	73929	74692	71589	74464	517901	441575	73595.83	6.48	1.047
21	93239	15001	14127	13615	15512	14752	14119	16004	103130	88129	14688.17	6.22	1.106
22	306574	46839	46155	45548	47172	45993	46490	47024	325221	278382	46397.00	6.55	1.061
23	59284	10064	9815	10035	10550	10413	9914	9829	70620	60556	10092.67	5.89	1.191
24	104953	17269	16898	17171	16635	16987	17274	17253	119427	102218	17036.33	6.10	1.138
25	161982	26298	25874	24149	27442	24657	26643	25173	180236	153938	25656.33	6.16	1.113
26	380008	59569	55972	59028	58539	57088	61172	60866	412234	352665	58777.50	6.38	1.085
27	525200	75738	81500	82629	82192	77823	78571	75525	554178	478440	79740.00	6.93	1.055
28	2758660	423039	412906	415273	407223	404738	413875	413209	2895263	2472224	412037.33	6.52	1.050
29	161189	27627	26372	27197	26113	26247	25802	26684	186042	158415	26402.50	5.83	1.154
30	342577	55313	53318	54004	56731	51130	51464	54616	378576	323263	53877.17	6.19	1.105
31	474610	74096	71701	74394	71943	69395	72578	76583	511690	437594	72932.33	6.41	1.078
32	315374	49359	48256	47361	50374	48418	46038	47976	337782	288423	48070.50	6.39	1.071
33	300238	46603	44107	45881	45782	44034	44752	46372	317531	270928	45154.67	6.44	1.058
34	526536	76812	78414	81315	80042	75916	79707	81756	553962	477150	79525.00	6.85	1.052
35	663595	105471	105038	93340	98366	99325	94265	94747	690552	585081	97513.50	6.29	1.041
36	26386	5514	4971	4284	4534	4650	5171	4276	33400	27886	4647.67	4.79	1.266
37	53515	9654	9055	8992	9146	8801	8999	9294	63931	54277	9046.17	5.54	1.195
TOT	10188042	1602390	1570651	1564547	1568754	1538195	1560933	1569694	10975164	9372774	1562129.00	6.36	1.077

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