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Lecture Notes in Mathematics

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PREFACE

This volume contains a collection of special invited lectures on computational methods in nonlinear mechanics prepared by specialists from a wide collection of disciplines. With the exception of Chapter 2, all of these lectures were also delivered at the International Conference on Computational Methods in Nonlinear Mechanics held in Austin, Texas, in September 1974, which was held under the sponsorship of the U. S. National Science Foundation. The original intention of the meeting, and for collecting this set of lectures, was to bring together in one place the latest results on computational methods for nonlinear problems from a number of diverse areas in the hope that techniques that had been found successful in one area may have some impact on problems in other areas. In addition, it was hoped that the state-of-the-art in certain areas of computational mechanics could be summarized. I believe that a reader who examines the contents will agree that both of these objectives have been accomplished.

J. T. Oden
Austin, 1975

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BILATERAL ALGORITHMS AND THEIR APPLICATIONS

W. F. Ames and M. Ginsberg

1.1 Introduction. In this paper, algorithms providing iterative improvable upper and lower bounds are constructed for certain classes of nonlinear ordinary and partial differential equations arising in transport phenomena. Developments are based upon the construction of antitone functional operators which are oscillatory contraction mappings. Following the mathematical details, which include sketches of convergence and uniqueness proofs, several examples will be presented. Application of the general results will be made to nonlinear diffusion, non-Newtonian (power law) boundary layer flow and to diffusion with a generalized radiation condition.

1.2 Preliminary Definition. Let R and R* be partially ordered metric spaces and T be an operator whose domain $D \subseteq R$ and range $W \subseteq R^*$. Then T is said to be syntone if $v \le w$ implies $Tv \le Tw$ for every $v, w \in D$ and strictly syntone if $v < w$ implies $Tv < Tw$. T is said to be antitone if $v \le w$ implies $Tv \ge Tw$ for every $v, w \in D$. T is monotone if it is either syntone or antitone.

A bilateral or error bounding algorithm for the solution of an operator equation produces a sequence of approximate solutions such that the true solution is bounded between every pair of successive approximations.

1.2.1 Introductory Example. As a motivation for what follows consider the elementary nonlinear equation

$$\frac{dy}{dt} = -y(y - 2) \quad , \quad y(0) = 1 \tag{1.1}$$

the exact solution of which is

$$y(t) = 2/[1 + \exp(-2t)] \tag{1.2}$$

Problem (1.1) is convertible to the operator form $y = Ty$, from which successive approximations $y_n = Ty_{n-1}$ can be developed, in a variety of ways. If the classical Picard procedure is employed (1.1) becomes

$$\frac{dy_n}{dt} = -y_{n-1}(y_{n-1} - 2), \qquad y_n(0) = 1 \tag{1.3a}$$

and the integral form is

$$y_n = 1 - \int_0^t y_{n-1}(y_{n-1} - 2)\, dt \tag{1.3b}$$

As a first alternative a Newton-Picard approximation to (1.1) gives

$$\frac{dy_n}{dt} + 2[y_{n-1} - 1]\,y_n = y_{n-1}^2 \quad , \quad y_n(0) = 1 \tag{1.4a}$$

with the associated integral form

$$y_n = \left[\exp\left[-2\int_0^t (y_{n-1} - 1)ds\right]\right]\left[\int_0^t y_{n-1}^2 \exp\left[2\int_0^s (y_{n-1} - 1)dr\right] ds + 1\right] \tag{1.4b}$$

Lastly an approximation which leads to a Bilateral algorithm, as will be subsequently demonstrated, carries (1.1) into

$$\frac{dy_n}{dt} = -y_n(y_{n-1} - 2) \quad , \quad y_n(0) = 1 \tag{1.5a}$$

with the integral form

$$y_n = \exp\left[-\int_0^t (y_{n-1} - 2)\,ds\right] \tag{1.5b}$$

Clearly, (1.3b), (1.4b) and (1.5b) all have the form $y_n = Ty_{n-1}$ but the properties and complexities of the operators are vastly different. Since direct comparison is not the present purpose only the properties of (1.5b) will be briefly examined.

If it is assumed that $y_{n-1} < y_n$ then it follows from (1.5b) that

$$y_n = \exp\left[-\int_0^t (y_{n-1} - 2)\,ds\right] > \exp\left[-\int_0^t (y_n - 2)\,ds\right] = y_{n+1}$$

that is $y_n > y_{n+1}$ and (1.5b) is antitone. By an analogous argument if it is assumed that $y_{n-1} > y_n$ then $y_n < y_{n+1}$. From (1.5b) it follows that each iterate is positive. Thus, beginning with $y_1 = 0$ it follows that $y_1 < y_2$. By application of (1.5b) the following inequalities result:

$$y_1 < y_2 \quad , \quad y_3 < y_2 \quad , \quad y_3 < y_4 \quad , \quad y_5 < y_4 \quad , \quad \ldots \tag{1.6}$$

Since y_1 y_3 the following inequalities result:

$$y_1 < y_3 \quad , \quad y_4 < y_2 \quad , \quad y_3 < y_5 \quad , \quad y_6 < y_4 \quad , \quad . . . \tag{1.7}$$

As a consequence of the foregoing analysis the even subsequence $\{y_{2n}\}$ is seen to form a monotonic decreasing sequence of upper bounds to the exact solution. Since it is bounded below the subsequence has a limit y_E. The odd subsequence $\{y_{2n+1}\}$ forms a monotonic increasing sequence of lower bounds to the exact solution. It is bounded above since every odd term is less than all the even terms. Hence the odd subsequence has a limit y_0. Upon proof (deleted here) of uniqueness and convergence to the solution of the original problem a bilateral algorithm has been established. Moreover an estimate of the absolute error, at any step of the exact iteration, can be made from $|y_n - y_{n-1}|$. Further discussion of error analysis will be given subsequently.

The bilateral algorithm (1.5b), for problem (1.1), has been carried out numerically by Ginsberg [1]. Implementation for the computer was accomplished by using truncated Chebyshev polynomial approximations for the integral of (1.5b). Such approximations are found in practice to be "close" to minimax approximations. Some of the results and comparisons with the exact solution (1.2) are shown in Table 1.1. The convergence is very rapid, requiring two iterates (after $y_0 = 0$) at x = 0.25 and four at x = 1.00.

1.3 <u>Literature and Applications</u>. In this section, some literature and applications are reviewed.

1.3.1 <u>Some Applications</u>. Even though bilateral algorithms have not been readily available a number of applications appear in the literature. An early application is due to Weyl [2] (see also Ames [3]) who studied the Blasuius problem

$$f''' + ff'' = 0 \quad , \quad f(0) = f'(0) = 0 \quad , \quad f'(\infty) = 2 \tag{1.8}$$

by means of what is now called a bilateral algorithm. Barnov [4] reports that nonlinear differential equations representing flexural and torsional vibration of beams or buckling of rods often cannot be easily solved either analytically or by existing numerical methods in such a way that the positional relationship between the approximate and exact solutions is accurately revealed. A bilateral approach is helpful here; Baranov has developed such a method for his specific equations. In naval warfare problems involving the use of the Lanchester equations, Fabry [5] has defined a two-sided bounding scheme which offers a means of studying variations of certain parameters before the equations are solved by some conventional (nonbounding) method.

TABLE 1.1

BILATERAL SOLUTION FOR $y' = -y(y-2)$, $y(0) = 1$

analytic solution	lower bound	upper bound
x = 0.25	1.193885941790505	1.648710209585520
y = 1.244918662403709	1.244302764859383	1.249093098984541
x = 0.50	1.149627182408467	2.718291858828761
y = 1.462117157260010	1.452979881956689	1.526855263664362
x = 0.75	0.786591951891501	4.481684580133818
y = 1.635148952387287	1.556515566491166	1.964470533182715
	1.632492411677624	1.650773795468340
x = 1.00	0.3028473400060250	7.389056098930645
y = 1.761594155955765	1.427162894608360	2.831261923857015
	1.737914377152946	1.862242176203166
	1.760705861515525	1.766475649019048

NOTE: These results are obtained from the program of Ginsberg [1]. The halting criteria consisted of a check every two iterations which used $(n+1) \times 0.5 \times 10^{-15}$ as a bound on roundoff error and $\max(|a_{n-1}|, |a_n|, |a_{n+1}|)$ as a bound on the truncation error. For each iteration 9 terms ($n = 8$) are used in each Chebyshev expansion.

Boley [6] has used a bilateral approach for problems of heat conduction in melting or solidifying slabs; his work can also provide approximations for certain types of aerodynamic ablation problems. Appl and Hung [7] have applied a two-sided technique to continuous equilibrium problems such as a fin temperature problem in which there is internal heat generation. Ispolov and Appl [8] have employed a bilateral method for a problem of self-sustained vibration of an autonomous system. Kahan [9,10] has developed an ellipsoidal bounding technique which can be applied to the N body problem. Two-sided bounding methods have also been employed by Weinstein and Stenger [11] for problems involving vibrations of cantilever plates or energy levels in quantum mechanics. Mann and Wolf [12], Roberts and Mann [13], Padmavally [14], Friedman [15], Levinson [16] and Keller and Olmstead [17] treat various aspects of heat conduction with a nonlinear (radiative) boundary condition and associated problems. A major factor in all of these works is the conversion to an integral equation whose solution by successive approximations generates a bilateral scheme.

1.3.2 <u>General Literature for Initial Value Problems</u>. In this general literature review attention is confined to bilateral techniques which can be employed on initial value problems. Special attention is paid to procedures which are iteratively improvable.

Chaplygin [18,19] and others (see Azbelev [20], Babkin [21,22], and Gendzhoyan [23]) have worked with differential inequalities which have led to bilateral methods; however, most of their results apply to very specialized problems. No attempts seem to have been made to implement any of these techniques for automatic computation. This is most likely the case because these schemes are generally awkward to work with and their inherent analytical nature is not very amenable to a computer implementation. Furthermore, most variations of Chaplygin's results require replacement of the original problem with <u>two</u> new problems, one with a solution above that of the original problem and one with a solution below. Thus, any computerized version of such a method would most likely require considerably more computational effort than would the application of a more conventional (nonerror bounding) method to the original problem.

An interval analysis approach developed by Moore [24,25] and associates (Braun and Moore [26], Krückeberg [27], and Reiter [28]) produces upper and lower bounds to the solution of certain restricted classes of scalar and vector first order initial value problems (as well as for a variety of other numerical analysis problems). This technique utilizes interval representations of terms in truncated Taylor series expansions. Unfortuately, the bounds generated by interval analysis tend to increasingly deviate from the exact solution as the computation progresses; thus, they can become very large unless sufficient backtracking is performed along with the introduction of additional terms in the Taylor series expansions. The process can be very time consuming for large vector problems. Moore [24] indicates that the inherent nature of his approach will often produce some unduly conservative (large) bounds, regardless of the variations employed in the computer implementation. He suggests that one possible remedy to this dilemma would be to utilize multiple precision computation. Regretably, such action could significantly increase the program's execution time and/or its memory requirements. Some variations of Moore's original method are under development (e.g. see Krückeberg [27]) and it is hoped that some of the above-mentioned difficulties may be overcome. Also future compiler aids as well as microprogramming and/or hardware assistance may alleviate a significant portion of the computational overhead costs which have prevented widespread use of interval analysis for complicated engineering problems.

Interval analysis has stimulated the creation of a new method developed independently by Kahn [9,10] and Guderley and Keller [29,30]. Whereas the bounds generated by interval analysis form rectangular parallelpipeds which enclose the exact solution, the new technique defines an ellipsoid which contains the exact solution. Preliminary results indicate that ellipsoidal bounds can be more precise and require less computational effort (in large vector problems) than their interval analysis counterparts. The approach is still in a relatively early stage of development; its potential usefulness has probably not yet been fully realized.

There have been a few other attempts to create bilateral methods but most of them seem to apply only to very specific cases and/or are not readily adaptable for efficient and reliable computer implementation. Bulirsch and Stoer [31] have created extrapolation techniques which can produce a sequence of monotone upper and lower bounds to the exact solution of certain initial value problems; however, these bounds can only serve as good guesses and are not very precise because they are asymptotically true. Gorbunov and Shakhov [32] have produced modified Runge-Kutta algorithms with two-sided bounds; each bound requires the evaluation of a separate formula. The introduction of a significant number of parameters quickly complicates their procedure if very accurate bounds are desired. Each of their methods offers no iterative improvement, i.e. only one upper and lower bound are produced for each x value; one of their computational results is given in Ginsberg [1]. Fabry's [5] nested bound approach for Lanchester equations requires the user to specify good initial upper and lower bounds in order to assure convergence to the true solution. Also two new systems of differential equations must be solved for each pair of upper and lower bounds, thus decreasing the feasibility of performing very many iterations.

A functional operator approach involving syntone, anitone, and monotone decomposable operators has been discussed by Collatz [33,34]. Applications by Tal [35] and Berman and Plemmons [36] have produced bilateral bounds for systems of algebraic equations. T is a <u>monotone decomposable</u> operator if $T = T_1 + T_2$ where T is represented by the sum of a syntone operator and an antitone operator, respectively, where T_1 and T_2 are continuous and have the same domain, D. Collatz [34] indicates that if given $v_0, w_0 \in D$, $[v_0, w_0] \subset D$ where

$$v_{n+1} = T_1 v_n + T_2 w_n$$

$$n = 0,1,2,\ldots$$

$$w_{n+1} = T_1 w_n + T_2 v_n$$

$$y' = f(x,y)$$

$$y = T(y(x)) = (T_1 + T_2)\ (y(x)) \tag{1.9}$$

for T_1 isotone and T_2 antitone, then

$$v_0 \le v_1 \le v_2 \le \ldots \text{ exact solution } \ldots \le w_n \le \ldots \le w_2 \le w_1 \le w_0$$

Collatz does not attempt to establish this method for any large classes of differential equations. This approach seems worthy of further investigation to determine the extent of applicability.

Davis and James [37] (see also Ames [3]) have reported on a bilateral algorithm employing an antitone operator for the scalar initial value problem

$$y' = -\, y f(x,y) \tag{1.10}$$
$$y(x_0) = \beta > 0\ .$$

where in a range R: $x_0 < x < x_0 + h$ for $h > 0$:

a) The exact solution, $y(x)$, and $f(x,y)$ are strictly positive for $x \in R$ and are bounded for values in R.
b) $f(x,y)$ is a monotonically increasing function of y, i.e. if $y_1 \le y_2$ then $f(x,y_1) \le f(x,y_2)$.
c) $f(x,y_1) - f(x,y_2) < K(y_1 - y_2)$ for constant $K > 0$.

Then the iterates defined by

$$y_n(x) = \beta \exp\left[-\int_{x_0}^{x} f(u,y_{n-1}(u))\,du\right] \tag{1.11}$$

converge to the exact solution, $y(x)$, monotonically from above and below for every $x \in R$,

$$y_1(x) < y_3(x) < \ldots < y_{2n+1}(x) < \ldots < y(x) < \ldots < y_{2n}(x) < \ldots < y_4(x) < y_2(x).$$

The preliminary example presented in Section 1.2.1 is of this type as is the work of

Weyl [2] who developed an operator form for the second derivative. A generalization of the result of Davies and James will be given subsequently.

Two-sided approaches have also served as a device for establishing existence and uniqueness of solutions. In fact the Davies and James [37] approach is primarily for that purpose. Indeed the works of Mann and Wolf [12], Roberts and Mann [13], Padmavally [14], Friedman [15], Levinson [16], and Keller and Olmstead [17] provide just such proofs on the way to establishing other properties for their problems. Gendzhoyan [23] employed Chaplygin's concepts for his study of existence and uniqueness of a boundary value problem.

Substantial additional material concerning the literature and a summary of the methods can be found in Ginsberg [1].

1.4 Generalization of the Weyl-Davies-James Method. Davies and James [37] observed that a slight modification of Picard's method produces oscillatory convergent iterates for some scalar differential equations. Their result is a special case of a theorem presented in Section 1.4.1. Following a sketch of the proof several examples will be given. The proof employs concepts from fixed point theory. Before proceeding, a few definitions and known results (Rall [38]) are given.

Definition 1.4.1: If $z = F(z)$ for some z belonging to a Banach space Q on which operator F is defined as an into mapping, then z is said to be a fixed point of the operator F.

Definition 1.4.2: An operator F defined as an into mapping on a Banach space Q, with norm $\| \ \|$, is called a contraction mapping of the closed region $\overline{U}(y_1,r) \equiv \{y: \|y - y_1\| \le r \text{ for some } r > 0\}$ if there exists a positive number θ, $0 \le \theta < 1$ such that $\|F(s) - F(t)\| \le \theta \|s - t\|$ for every $s,t \in \overline{U}(y_1,r)$.

Theorem 1.1 (Rall [38]) (Contraction Mapping Theorem). Let F be an operator on a Banach Space Q, with norm $\| \ \|$. Suppose F is a contraction mapping of $\overline{U}(y_1 r)$ where $r \ge \frac{1}{1-\theta} \|y_1 - F(y_1)\| = r_1$. Let the sequence $\{y_n\}$ be defined via $y_{n+1} = F(y_n)$, $n = 1,2,3,\ldots$. Then F has a fixed point $y^* \in \overline{U}(y_1,r_1)$ which is also the unique fixed point of F in $\overline{U}(y_1,r)$ to which the sequence $\{y_n\}$ converges and $\|y_n - y^*\| \le \theta^{n-1} r_1$.

One natural question which arises from examining Theorem 1.1 is the following: Is there an upper bound on the distance (measured in the norm of Banach space Q) that the initial iteration y_1 can be from the fixed point y^* and still insure convergence of the sequence of iterates, $\{y_n\}$, to that fixed point? The answer to this question depends on the region in which the contraction mapping holds. Theorem 1.1 demonstrates that if y_1 can be defined as the center of a closed contraction mapping region $\overline{U}$ with radius $\ge r_1$, then it does not matter how far y_1 is from y^*. Furthermore, it can be shown (Rall [38]) that if the contraction mapping holds for the entire Banach space Q, then an extension of Theorem 1.1 can establish the existence and uniqueness of the fixed point y^*. In this situation y_1 can be any point in Q for which $F(y_1)$ is defined.

Thus in selecting y_1 it is necessary to have some a priori knowledge of the region in which the contraction mapping holds. Of course, the distance between y_1 and the fixed point can affect the number of iterations required to satisfy a certain convergence tolerance (the exact extent of this effect is dependent on other specified characteristics of the operator F).

Since Theorem 1.1 plays a major role in the proof of Theorem 1.2 it will follow that these observations about the selection of y_1 will also apply to this general theorem and to the variations which will be presented later.

1.4.1 A Generalization. Consider the initial value problem

$$y' = g(y)\, f(x,y) \quad , \quad y(x_0) = \beta > 0 \tag{1.12}$$

where g is such that the operator G, defined via

$$G(u) + C = \int \frac{du}{g(u)} \qquad \text{(C constant)} \tag{1.13}$$

is a continuous operator on the space of differentiable functions D, G^{-1} exists as a strictly positive antitone continuous operator on D and (1.12) has a strictly positive solution y(x), for every x, $x_0 \le x \le x_0 + h$, $h > 0$. Further suppose f(x,y) has the following properties:

a) f(x,y) is strictly monotone increasing function of y;

b) $0 < f(x,y) < M$ for every x, $x_0 \le x \le x_0 + h$;

c) f satisfies a weakened Lipschitz condition on a closed region about y_1 denoted by $\overline{U}(y_1,r) \equiv \{y: \|y - y_1\| \le r,\ r > 0\}$; that is $f(x,\xi_1) - f(x,\xi_2) < K(x)(\xi_1 - \xi_2)$, $\xi_1 > \xi_2$ for every ξ_1, $\xi_2 \subset \overline{U}(y_1,r) \subset D$ and for $< K(x) < N$, for every x, $x_0 \le x \le x_0 + h$.

Theorem 1.2. Let the preceding assumptions be satisfied. Then there is a sequence of positive iterates $\{y_n\}$ satisfying

$$\frac{dy_n}{dx} = f(y_n)\, f(x,y_{n-1}) \tag{1.14}$$

$$y_n(x_0) = \beta > 0 \quad , \tag{1.15}$$

where

$$y_n(x) = G^{-1}\left[\int_{x_0}^{x} f(u,y_{n-1}(u))\, du + G(\beta)\right] \tag{1.16}$$

Further, the sequence $\{y_n\}$ is such that

$$y_1(x) < y_3(x) < \ldots < y_{2n-1}(x) < \ldots < \ldots < y_{2n}(x) < \ldots < y_4(x) < y_2(x)$$

for every x in $x_0 \le x \le x_0 + h$. The sequence has a limit function $y(x)$ which satisfies the initial value problem (1.12).

To establish the successive approximation (1.16), Equation (1.12) is rearranged and integrated. Development of the order relationships amongst the even and odd iterates follows from the two relations

$$\begin{aligned} y_{n-1} < y_n \quad &\text{implies} \quad y_{n+1} < y_n \\ y_{n-1} > y_n \quad &\text{implies} \quad y_n < y_{n+1} \end{aligned} \tag{1.17}$$

If it is assumed that $y_{n-1} < y_n$ then

$$f(x,y_{n-1}) < f(x,y_n)$$

since f is strictly monotonic increasing. Consequently

$$\int_{x_0}^{x} f(u,y_{n-1}(u))\,du + G(\beta) < \int_{x_0}^{x} f(u,y_n(u))\,du + G(\beta)$$

whence

$$y_n = G^{-1}\left[\int_{x_0}^{x} f(u,y_{n-1}(u))\,du + G(\beta)\right] > G^{-1}\left[\int_{x_0}^{x} f(u,y_n(u))\,du + G(\beta)\right] = y_{n+1}$$

since G^{-1} is strictly antitone. The second relation of (1.17) is developed in a similar fashion. Let $y_1 = 0$. Since $0 < G^{-1}(\xi)$ for every ξ in D it follows that all y_i, $i > 1$, defined by (1.16) are positive.

Now G^{-1} must be shown to be a contraction mapping to justify the application of Theorem 1.1. To this end write (1.16) as

$$y_n = G^{-1}(y_{n-1}) \quad , \quad n = 2,3,\ldots \tag{1.18}$$

where G^{-1} is defined on

$$\overline{U}(y_1,r) = \{y: \ \|y - y_1\| \le r \quad , \quad \text{some } r > 0\} \subset D \ .$$

Using the weakened Lipschitz condition it then follows by an indirect proof that