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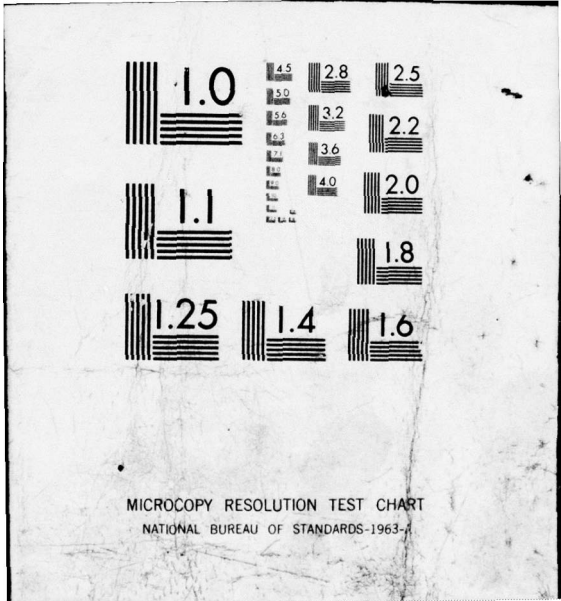
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A MULTIPLE SHOOTING AND SWEEP ALGORITHM  
FOR OPTIMAL POINT CONTROLLED  
DISTRIBUTED PARAMETER SYSTEMS

B. J. Olufeagba, R. H. Flake  
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ABSTRACT

The solution of the sparse algebraic system for a point controlled elliptic distributed parameter system by a multiple shooting and sweep algorithm is discussed. The multiple shooting and sweep algorithm enhances the convergence rate of the ordinary shooting method while achieving a significant reduction in the dimension of the linear equations to be solved.

The optimization algorithm for a special problem involving the minimum cost selection of source intensities with the state satisfying a specified constraint set is presented. An application of the techniques involving the analysis and management design for water quality control in Corpus Christi Bay, an estuary on the Texas Gulf Coast in the United States, is discussed. The resulting algorithm is more than twice as fast as a corresponding successive overrelaxation method.

INTRODUCTION

The control of a class of distributed parameter systems which are described by elliptic partial differential equations specified over a two dimensional spatial domain and satisfying mixed Dirichlet and Neumann type boundary conditions (1) is considered. The controls for the system are defined by parameters whose influence is exerted pointwise. Systems of this type are encountered for example in estuarine water quality problems (2) where the point controls correspond to pollution discharges into estuaries.

A method of solving the finite difference approximation for the boundary value problem based on a multiple shooting (3) technique is presented. It is equivalent to a Newton's solution of the system equations generated when the boundary value problems are re-expressed as initial value problems. The method, which converges for the elliptic system, has been demonstrated to achieve convergence in two example problems after less than 10 iterations

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and is more than twice as fast as the corresponding successive over-relaxation (SOR) solution methods (4, 5). The order of linear algebraic equations to be solved is the maximum of  $N$  or  $M$  where,  $N$  and  $M$  are the number of grid points defined in the coordinate directions for the approximate problem. This compares favorably with the  $N \times M$  order system usually required in the other methods.

The determination of optimal cost removal policies for discharges by nonlinear programming is discussed when the spatial concentration defined by the system equations are required to satisfy a set of state variable inequality constraints. The sensitivity for the system state to the parametric controls is shown to satisfy a monotonicity condition. This monotonicity may be combined with convexity of the cost functions to reduce the order of the resulting nonlinear programming problem by solving a set of problems defined for relaxed consistent state variable constraints that converge to the desired constraints.

The solution technique is applied to a study of the spatial distribution of phosphorus in Corpus Christi Bay, which is a large shallow estuary on the Texas Coast. The determination of the minimum cost of phosphorus treatment based on source projections for 1980 and the predicted hydrodynamics (4) of the bay are presented. The convergence of the method in the positive definite case was demonstrated by a simple ratio test for the sequence of initial value corrections generated by the shooting algorithm. The extension of this approach shows promise in the solution of boundary value problems in which more than one independent variable is considered.

Multiple Shooting Solutions of a Distributed System

The class of problems discussed here have a state equation given by an elliptic partial differential equation satisfying mixed Dirichlet and Neumann boundary conditions.

$$\frac{\partial}{\partial x} \left( E_x(x, y) \frac{\partial C}{\partial x} \right) + \frac{\partial}{\partial y} \left( E_y(x, y) \frac{\partial C}{\partial y} \right) - \frac{\partial}{\partial x} \left( u(x, y) C \right) - \frac{\partial}{\partial y} \left( v(x, y) C \right) - K(x, y) C = f(x, y, \alpha), \quad (x, y) \in \Omega \quad (1)$$

subject to boundary conditions

$$C(x, y) = \text{given} \quad (x, y) \in \partial \Omega_1, \text{ Dirichlet condition} \quad (2)$$

$$Q \cdot n = 0 \quad (x, y) \in \partial \Omega_2, \text{ Neumann condition} \quad (3)$$

where  $C(\dots)$  - state variable

$E_x(x, y), E_y(x, y) \in C^{1,1}(\Omega)$  - dispersion coefficients in the coordinate directions,  $E_x, E_y > 0, \forall (x, y) \in \Omega$

$f(x, y, \cdot)$  - control functions

$K(x, y)$  - reaction rates

$n$  - outward pointing normal on the boundary

$$Q = - \left[ (u C - E_x \frac{\partial C}{\partial x}), (v C - E_y \frac{\partial C}{\partial y}) \right]$$

$u(x, y), v(x, y)$  - velocity coefficients in the coordinate directions

$(x, y)$  - independent variables

$\alpha$  - control parameters,  $\alpha \in R^m$

$\Omega$  - simply, connected open region,  $\Omega \subset R^2$

$\partial \Omega = \partial \Omega_1 \cup \partial \Omega_2$  - boundary of region  $\Omega$

If in addition to the conditions specified above, the equations satisfy an ellipticity condition (1), then there exists a unique solution

$$C(x, y) \in C^{2,2}(\Omega).$$

Furthermore, the problem is well-posed with respect to the initial data in the sense of Hadamaard (6).

The solution technique discussed in this paper is based on reformulating the boundary value problem as an initial value problem. Although the resulting initial value problem violates the Hadamaard condition, a special variant of multiple shooting is employed to improve convergence and generate the initial conditions compatible with the specified data and the solution.

### Multiple Shooting Solutions

For simplicity consider the pure Dirichlet problem defined on a convex region  $\Omega$ . Define a partition in the y-coordinate direction and approximate the derivatives along the partitioned coordinate axis. The approximation,  $C_j(x)$ , then satisfies the two-point boundary value problem defined for a set of coupled second order ordinary differential equations

$$\frac{\partial}{\partial x} \left( E_x^j(x) \frac{\partial C_j}{\partial x} \right) - \frac{\partial}{\partial x} \left( u_j(x) C_j \right) - \left[ C_{j+1} \left( \frac{E_{j+\frac{1}{2}}}{\Delta y^2} - \frac{2V_{j+1}}{\Delta y} \right) - C_j \left( \frac{E_{j+\frac{1}{2}} + E_{j-\frac{1}{2}}}{\Delta y^2} - K \right) - C_{j-1} \left( \frac{E_{j-\frac{1}{2}}}{\Delta y^2} - \frac{2V_{j-1}}{\Delta y} \right) \right] = f(x, y_j, \alpha) \quad (4)$$

where  $j=1, 2, 3, \dots, m, x \in (x_{j\min}, x_{j\max})$

subject to boundary conditions

$$C_j(x_{j\min}) = \text{given}$$

$$C_j(x_{j\max}) = \text{given} \quad (5)$$

where

$x_{j\min}$  - x coordinate for the beginning of the jth filament

$x_{j\max}$  - x coordinate for the end of the jth filament

$\Delta y$  - space mesh

$$E_{j+\frac{1}{2}} = E(x, (j+\frac{1}{2}) \Delta y)$$

$$V_{j+1} = V(x, (j+1) \Delta y)$$

The above equations (4) may be rewritten in a blocked matrix form as follows

$$\begin{bmatrix} \frac{\partial C_j^*}{\partial x} \\ \frac{\partial W}{\partial x} \end{bmatrix} = \begin{bmatrix} 0 & I \\ A & D \end{bmatrix} \begin{bmatrix} C^* \\ W \end{bmatrix} \quad (6)$$

where

$$C^* = [C_1(x), \dots, C_m(x)]^T$$

$$W = \left[ \frac{\partial C_1(x)}{\partial x}, \dots, \frac{\partial C_m(x)}{\partial x} \right]^T$$

A = tridiagonal matrix dependent on the coefficients

$$D = \text{diag} [\delta_1, \delta_2, \dots, \delta_m]; \delta_j = (u_j(x) - \frac{\partial E_j^j(x)}{\partial x})$$

I = m x m identity matrix

subject to the boundary conditions

$$C^*(0) = \text{given}$$

$$C^*(x_{\max}) = \text{given} \quad (7)$$

The problem is a linear two point boundary value problem, which in the ideal case can be solved by shooting methods (3, 7). The instability of the initial value problem for the elliptic system remains and is manifested by the rapid growth of the trial solutions (7) made with incorrect initial conditions.

Let the missing initial values be designated by

$$g_j = W(x_{\min, j}), \quad j = 1, 2, 3, \dots, m$$

Then, the shooting solution corresponds to Newton's solution for a linear algebraic system

$$\xi(g) = \Phi(g - g^*) \quad (8)$$

where  $\Phi$  is the Jacobian matrix,  $\Phi_{ij} = \frac{\partial \xi_j}{\partial g_i}$

g - arbitrary initial value vector,  $g \in R^m$

$g^*$  - initial value vector corresponding to the solution satisfying the boundary conditions

$\xi_j$  - the deviation; between specified and calculated terminal conditions at the boundary points given by

$$\xi_1 = C^*(x_{\max}, g^*) - C^*(x_{\max}, g)$$

The sequence of iterates is determined by the formula

$$g^{(n+1)} = g^{(n)} - \Psi^{-1} \xi(g^{(n)}) \quad (9)$$

where  $g^{(0)}$  is arbitrary.

In the ideal situation, then

$$\Psi = \Phi$$

and the algorithm converges in one step.

In practice, the shooting algorithm generates a sequence of iterates  $\{g^{(n)}\}$ , which is convergent if the matrix  $\Psi$  is positive definite and if

$$\|\Psi^{-1} \Phi - I\|_{\infty} < 1 \quad (10)$$

Due to the growth of trial solutions, condition (10) may not be satisfied and the ordinary shooting algorithm would consequently fail to converge. The effect of the excessive growth is usually manifested by the loss of significant figures in the trial solutions but it may be reduced by multiple shooting (3, 7, 8) methods. For multiple shooting, the strips  $(x_{\min, j}, x_{\max, j})$  may be partitioned into subintervals

and numerous alternative multiple shooting strategies may be implemented. The size of the subintervals is chosen to optimize computational accuracy and enhance the convergence of the shooting algorithm. Although the dimension of the initial value vector, g, is increased by multiple shooting, the Jacobian matrix is very often sparse and may be inverted rapidly by special algorithms. The method will be illustrated by a practical example, where the initial value problems are solved by a simple modified Euler numerical integrator such that the resulting equations are equivalent to ordinary finite difference approximation of the problem. The order of the Jacobian for the multiple shooting solution technique is still considerably less than the finite difference approximation matrix and achieves the same order of convergence accuracy in less than half the computational time of the successive over-relaxation (4) method and in about one hundredth the number of iterations. This method has several promising extensions such as the variable-metric multiple shooting technique, which eliminates the need to invert the Jacobian (9). The applications of multiple shooting combined with special fixed step/variable step numerical integrator schemes also provides a method of decreasing the truncation errors in the numerical approximations

of the state equations.

Point Control and Optimization

An important design problem involves the selection of constrained control parameters  $\alpha$ , which achieve some specified goal at minimum cost, where the goals are assumed to lie within the reachable set of the admissible region. The problems of this type can be formulated as the minimization of a convex cost function subject to linear constraints. The linear constraints are determined from the sensitivity functions to the  $\alpha$  parameters and constitute part of a nonlinear programming solution. The large dimensionality of the constraints is reduced by exploiting some of the special qualities of the sensitivity functions which we derive below.

The control problem may be formulated as follows

Find

$$\inf_{\alpha \in \mathcal{B}} J(\alpha) : J(\alpha^*) \leq J(\alpha), \forall \alpha \in \mathcal{B} \quad (11)$$

subject to the constraints equation (1), (2) and (3)

where

$\mathcal{B} \subset \mathbb{R}^n$ , is a convex set of control parameter

constraints and such that

$$C(x, y) \leq g(x, y)$$

where for simplicity it is assumed that the function  $g(x, y) \in H(\mathcal{B})$ , the reachable set for the parameter control, and the cost functional  $J(\cdot)$  are assumed to be convex. The problem defined above may be reformulated as follows:

Find

$$\inf_{\alpha \in \mathcal{B}} J(\alpha)$$

subject to constraints.

$$C_0(x, y) + S_\alpha \cdot \alpha = C(x, y) \leq g(x, y) \quad (11a)$$

where  $S_\alpha$  is the sensitivity function (10) matrix (vector)  $\frac{\partial C}{\partial \alpha}$  which satisfies the problem

$$\begin{aligned} \frac{\partial}{\partial x} \left( E_x(x, y) \frac{\partial S_\alpha}{\partial x} + \frac{\partial}{\partial y} \left( E_y(x, y) \frac{\partial S_\alpha}{\partial y} \right) \right) - \frac{\partial}{\partial y} (u S_\alpha) \\ - \frac{\partial}{\partial y} (v S_\alpha) - K(x, y) S_\alpha = \frac{\partial f}{\partial \alpha}(x, y, \alpha), (x, y) \in \Omega \quad (12) \end{aligned}$$

subject to boundary conditions.

$$S_\alpha(x, y) = \text{given}, (x, y) \in \partial\Omega_1 \quad (13)$$

$$\frac{\partial Q}{\partial \alpha} \cdot n = 0, (x, y) \in \partial\Omega_2 \quad (14)$$

where  $C_0(x, y)$  is the solution to (1), (2) and (3) for a reference  $\alpha$ . Assume that  $f$  is linearly dependent on the parameter vector  $\alpha$  then the sensitivity function  $S_\alpha$  satisfies a monotonicity condition outlined in Theorem 1.

Lemma (11): If  $f: D \rightarrow \mathbb{R}$  is continuous and the domain  $D$  is a compact subset of a topological space, then  $f$  attains its maximum and its minimum, i.e., there exists points  $x_1, x_2$  of  $D$  such that

$$f(x_1) = \inf_{x \in D} f(x) \text{ and } f(x_2) = \sup_{x \in D} f(x)$$

where  $\mathbb{R}$  is the set of all real numbers.

Theorem I:

Consider the point controlled distributed parameter system described by equations (1) and conditions (2) and (3) with  $K > 0$ . The sensitivity functions

$S_\alpha = \frac{\partial C}{\partial \alpha}$  depend monotonically on  $\alpha$  and

$$\text{Sgn} \{S_\alpha(x)\} = - \text{Sgn} \left\{ \frac{\partial f}{\partial \alpha} \right\} \quad (15)$$

provided that the sign of  $\frac{\partial f}{\partial \alpha}$  is either positive (or negative) everywhere

Proof:

The sensitivity function  $S_\alpha$  (10) can be shown to satisfy (12) and conditions (13) and (14). Multiply (12) by  $S_\alpha$  integrate over  $\Omega$  and applying Green's formula gives

$$\begin{aligned} - \int_{\Omega} \left( E_x \frac{\partial S_\alpha}{\partial x} \cdot \frac{\partial S_\alpha}{\partial x} + E_y \frac{\partial S_\alpha}{\partial y} \frac{\partial S_\alpha}{\partial y} \right. \\ \left. - S_\alpha \frac{\partial (S_\alpha u)}{\partial x} - S_\alpha \frac{\partial (S_\alpha v)}{\partial y} \right) dx dy \\ = \int_{\Omega} S_\alpha \frac{\partial f}{\partial \alpha} dx dy, \forall S_\alpha \in \mathcal{C}^{2,2}(\Omega) \quad (16) \end{aligned}$$

From the ellipticity of the system equations, the left side of (16) is less than zero, hence

$$\int_{\Omega} S_{\alpha} \frac{\partial f}{\partial \alpha} dx dy < 0 \quad (17)$$

Consider the special case when

$\frac{\partial f}{\partial \alpha} = h(x, y) \geq 0, \forall (x, y) \in \Omega$ , then equation (17) implies:

$$\int_{\Omega} S_{\alpha} dx dy = \int_{\Omega_p} S_{\alpha} dx dy + \int_{\Omega_N} S_{\alpha} dx dy \quad (18)$$

where  $\Omega_p = \{ (s, y) \in \Omega : S_{\alpha} \geq 0 \}$

$\Omega_N = \{ (x, y) \in \Omega : S_{\alpha} < 0 \}$

It is clear from equation (17) that  $\Omega_N \neq \emptyset$ .

Applying the Lemma to any subset of  $\Omega_p \subset \mathbb{R}^2$ , it is clear that  $S_{\alpha}$  attains a maximum and there exists points

$(x_0, y_0) \in \bar{\Omega}_p$  such that

$$\frac{\partial S_{\alpha}}{\partial x} = \frac{\partial S_{\alpha}}{\partial y} = 0 \text{ and } \frac{\partial^2 S_{\alpha}}{\partial x^2}, \frac{\partial^2 S_{\alpha}}{\partial y^2} \leq 0 \quad (19)$$

If the maximum occurs on the Neumann boundary, then from the condition (14) it follows that

$$\frac{\partial S_{\alpha}}{\partial v} = 0, \text{ where } v \text{ is the coordinate along the normal.}$$

Applying the Lemma to the one dimensional manifold given by  $\partial \Omega_2 \cap \Omega_p$  also gives (19).

Note that  $S_{\alpha} = 0$  on  $\partial \Omega_1$ .

Applying (19) to equations (12) and assuming that

$$\frac{\partial u}{\partial x}, \frac{\partial v}{\partial y} \text{ are small gives}$$

$S_{\alpha} < 0$  at  $(x_0, y_0) \in \Omega_p$ , which contradicts the assumption that  $(x_0, y_0) \in \Omega_p$ , hence  $\Omega_p = \emptyset$ .

Repeating the argument with the sign of  $g(x, y)$  reversed gives the result

$$\text{Sgn} \{ S_{\alpha}(x, y) \} = - \text{Sgn} \left\{ \frac{\partial f}{\partial \alpha} \right\} \quad (20)$$

Q. E. D.

The above result demonstrates the monotonicity of the sensitivity function for a very special class

of inputs, and the reachable set defined on the admissible region may be readily expressed as the range of the affine mapping (11a).

The result is very useful in the example problem because it provides a means of simplifying the optimization task and it also provides a method of identifying the domain of influence for different control sources in the spatial domain.

The approximate sensitivity functions  $S_{\alpha}(i, j)$  may be determined directly by solving the sensitivity equations (12) through (14) using a shooting algorithm similar to that used for the system state. An alternative solution technique employs numerical differentiation with respect to the parameters and determines the sensitivity functions from a series of numerical solutions of the original problem as follows:

**Step I:** Solve the system equations with nominal control and determine  $C^0(x, y)$ .

**Step II:** Repeat Step I,  $m_c$  times, each time perturbing one component of the control parameter and generate the set of solutions

$C^j(x, y), j=1, 2, \dots, m_c$ , where  $m_c$  is the member of controllable sources. Choose  $\Delta \alpha$ , the perturbation parameter to ensure that the change in the solutions is significantly more than the convergence criterion.

**Step III:** Calculate the influence matrix (vector)

$$S_{\alpha}^j(x, y) = \frac{C^j(x, y) - C^0(x, y)}{\Delta \alpha} \quad (21)$$

**Step IV:** The solution for small changes (or in the linear case) about the nominal control can be determined from

$$C(x, y, \alpha) = C(x, y, \alpha_0) + S_{\alpha}^T(x, y) \cdot (\alpha - \alpha_0) \quad (22)$$

The control problem may then be reformulated as the following nonlinear programming problem consisting of a (cost) performance index, linear inequality constraints and bounds.

$$\text{minimize } J(\alpha) \quad (23)$$

subject to

$$S_{\alpha}(x_1, y_1)(\alpha - \alpha_0) \geq g(x_1, y_1) - C_0(x_1, y_1) \quad (24)$$

where  $\alpha \in \mathcal{A}$ , the set of admissible parameters and  $(x_1, y_1)$  are the coordinates of the finite difference grid points

Although the number of constraints in (24) could be very large, a significant order reduction may be achieved by using a set of relaxed constraint functions  $g^h(x_i, y_i)$  instead of  $g(x_i, y_i)$ , where

$$g^h(x_i, y_i) \text{ tend to } g(x_i, y_i).$$

The above results are illustrated in the following water quality examples.

#### An Application of Multiple Shooting Models in Water Quality Analysis and Management

The computation of concentrations for water quality constituents in Corpus Christi Bay, (Figure 1) illustrates an important application of a multiple shooting solution for elliptic distributed parameter systems. Corpus Christi Bay is a large shallow estuary on the Gulf of Mexico coast of Texas with an approximate area of two hundred and sixty square miles. The two dimensional, time averaged hydrodynamic flow components  $u(x, y)$ ,  $v(x, y)$  in the bay, were determined in an earlier study (12). The point sources in this problem are pollution discharges from various industrial complexes located on or within the bay perimeter. The boundary conditions are specified by the observed (Dirichlet) concentrations at the Laguna Madre, Aransas Pass and Rockport inlets, (Fig. 1) and the no flow (Neumann) conditions at the barriers and land/water interfaces.

The numerical approximation technique utilized in this example is similar to that discussed earlier, however, the numerical integration is performed by using a second order approximation for equations (4). The resulting system is equivalent to the finite difference approximation defined on the grid shown in Figure 2. Numerous alternative shooting policies could be defined for this problem. The directions of the shooting computations used in the example are indicated in the diagram (Fig. 2). For the case illustrated, 32 initial and intermediate values, indicated as  $G_j$ 's on Fig. 2,

were necessary to completely reformulate the resulting system as an explicit initial value problem. A consistent set of terminal conditions indicated as T's on Figure 2 were determined by checking the continuity and consistency of the solutions when computed from different directions as indicated in Figure 2.

The system was solved for the phosphorus concentrations throughout the bay. The measured and calculated values at 16 observation points throughout the bay were compared. The phosphorus distribution corresponding to the minimum square error between observed and calculated values (Table 1) is shown in Fig. 3. The solution for the multiple shooting case was computed in less than 6 seconds on a CDC6600

computer system. The solution was achieved in six iterations when the convergence criterion was specified to be

$$\max |g_j^{(n)} - g_j^{(n-1)}| < 10^{-6}$$

The convergent algorithms were characterized by the property that the ratios

$$\frac{|g_j^{(n)} - g_j^{(n+1)}|}{|g_j^{(n-1)} - g_j^{(n)}|} \text{ were constant } (< 1). \text{ Attempted}$$

acceleration of the solution by extrapolation methods using the above ratios slowed convergence because of the effect of round off on the computations. The errors (Figure 4) can be seen to be reduced initially by a very large value of  $\approx 10^9$  and then by smaller factors and finally oscillations due to roundoff. The number of iterations required for similar accuracy for a method equivalent to the successive over-relaxation technique (4) was about five hundred and required about 14 seconds on the CDC6600 computer. It is clear from this study that multiple shooting methods are competitive with and in some cases better than other well known iterative methods. The advantages include the reduced dimension of the matrices to be solved, which in this example were solved by a standard linear equation subroutine. For larger problems, the solutions may be computed by combining a variable metric technique with the shooting method to eliminate some of the inversions or linear system solutions.

The resulting model can be used to evaluate treatment policies for the discharges into the estuary, and a typical water quality management problem may be stated as follows:

Determine the optimal phosphorus treatment policies at the sources for some target year in the future such that the total cost of keeping the water quality at 1969 levels is minimized. This problem may be equivalently stated as follows

$$\min_{\alpha \in J} J(\alpha) = \sum_{j=1}^M \text{Cost}(\alpha_j) \quad (25)$$

subject to

$$S_\alpha(i, j) \alpha \leq C_{1969} - C_0(i, j) \quad (26)$$

where the cost function for a chemical coagulation plant assuming a twenty year life is

$$\text{Cost}(\alpha_j) = 5 \times 10^4 k_1 Q^2 + 0.365 \times 10^4 k_3 Q^4 \text{ \$/year} \quad (27)$$

$$Q = \frac{\alpha_j Q_j}{\eta_j}$$

$$M = \text{number of controllable sources} \quad (11)$$

$$\eta_j = 0.93; k_1 = 0.098; k_2 = 0.90$$

$$k_3 = 5.45; k_4 = -0.03.$$

$$Q_j = \text{size of the } j^{\text{th}} \text{ controllable discharge}$$

where the indices  $i$  and  $j$  correspond to the grid point  $(x_i, y_j)$  and the  $j$ th source, and

$$\alpha_j = \{\alpha_j, j=1, 2, \dots, m_c; 0.01 \leq \alpha_j \leq 0.93\}$$

The parameter sensitivity function matrix for 1980 conditions incorporating source (4) and hydrodynamic projections for Corpus Christi Bay was determined by the numerical differencing algorithm. The sensitivity function to the source intensity for one of the pollution discharges is shown in Figure 5 and the percent difference between the concentrations predicted by the shooting models and the sensitivity model is shown in Figure 6. The approximate sensitivity functions in general satisfy the condition specified in equation (17), however, some of the functions were positive in the upper regions of the bay (Nueces Bay and River), where the positive definiteness of the operator was questionable. The sensitivity model is within 1% of the shooting model except in the small area representing Corpus Christi harbour where the convergence error for the shooting algorithm was larger than usual. The large error observed in the upper regions of the bay is due to loss of numerical accuracy due to the growth of the initial value solutions. This type of error can be eliminated by a shooting scheme involving shooting in the negative  $y$  direction starting at the Nueces/Corpus Christi Bay junction.

The optimal cost policy for the problem was determined by a version of Goldfarb's method for constrained nonlinear programming problems (13, 14). The number of inequalities in the constraint set (26) was reduced by solving a set of intermediate problems each defined by finding the optimal cost for correcting the worst fifty violations. The optimal treatment efficiencies at the controllable plants is achieved at a total cost of

\$264,000/year are as shown in Table 1 with the corresponding optimal profile shown in Figure 7. This corresponds to an overall savings of about ninety thousand dollars per year over the cost of maintaining total effluent discharges for the eleven controllable sources at the 1969 levels.

#### SUMMARY AND CONCLUSIONS:

A method of solving the sparse large linear approximations for point controlled elliptic distributed parameter systems by multiple shooting was discussed. The method was applied to the analysis of a water quality system with 264 elements. The linear system generated by the multiple shooting technique was a  $32 \times 32$  matrix with a large number of zero elements. Convergence was achieved in a few iterations at a speed twice that of a comparative successive over-relaxation algorithm for the same problem. A result about the sensitivity function of the control parameters was derived, which serves as a useful check for an alternative perturbation model for the problem. An analysis technique based on the shooting algorithm was employed to solve for the optimal management policies for controllable sources in Corpus Christi Bay. The method may be extended to solve even larger problems by a combination of multiple shooting with the variable metric methods which eliminate the need to solve large linear algebraic systems.

#### REFERENCES

- (1) J. L. Lions, Control of Systems Governed by Partial Differential Equations, Springer-Verlag, 1971.
- (2) J. W. Dalley and D. R. F. Harleman, Fluid Dynamics, Addison-Wesley Pub. Co., Reading, Mass., 1966.
- (3) S. M. Roberts and J. S. Shipman, Two Point Boundary Value Problems, Elsevier Pub. Co., Inc., 1972.
- (4) B. R. Penumalli, R. H. Flake, and E. G. Fruh, "Water Quality Modelling and Management Studies for Corpus Christi Bay: A Large Systems Approach," Center for Research in Water Resources, University of Texas at Austin, CRWR Report 122, 1974.
- (5) D. M. Young, Iterative Solution of Large Linear Systems, Academic Press, 1971.
- (6) P. R. Garbedian, Partial Differential Equations, John Wiley Pub. Co., 1967.
- (7) H. B. Keller, Two Point Boundary Value Problems, Academic Press, 1968.

- (8) D. D. Morrison et al, "Multiple Shooting for Two Point Boundary Value Problems," Comm. ACM 5, pp. 613-614, 1962.
- (9) B. J. Olufeagba and R. H. Flake, "A Variable Metric Method and Multiple Shooting for Analysis of Large Sparse Linear Systems," Research Proposal.
- (10) R. Tomovic, Sensitivity Analysis of Dynamic Systems, McGraw-Hill Book Co., Inc., 1963.
- (11) E. J. McShane and T. A. Botts, Real Analysis, pp. 71, D. Van Nostrand Co., Inc. 1959.
- (12) R. J. Brandes and F. D. Masch, "Tidal Hydrodynamics and Salinity Models for Corpus Christi and Aransas Bays, Texas," A report to the Texas Water Quality Development Board, Sept., 1972.
- (13) D. M. Himmelblau, Applied Nonlinear Programming, McGraw-Hill Co., 1972.
- (14) D. Goldfarb and L. Lapidus, "A Conjugate Gradient Method for Nonlinear Problems with Linear Constraints," Industrial and Engineering Chemistry Fundamentals, Vol. 7, pp. 142-151, (1965).

TABLE 1  
Observed and Calculated Long-Term  
Phosphorous Concentrations in Corpus Christi Bay

	Cell Location (i,j)	Observed Phosphorous Concentrations (mg/l)	Calculated Phosphorous Concentrations (mg/l)	Difference in mg/l
1	19,1	0.010	0.010	0.000
2	7,3	0.025	0.019	0.006
3	26,3	0.020	0.017	0.003
4	13,5	0.025	0.020	0.005
5	7,6	0.025	0.022	0.003
6	26,6	0.025	0.018	0.008
7	12,8	0.030	0.022	0.008
8	6,13	0.030	0.025	0.005
9	9,13	0.040	0.026	0.014
10	11,14	0.030	0.028	0.002
11	7,17	0.135	0.126	0.009
12	8,18	0.070	0.072	0.002
13	8,19	0.070	0.070	0.000

Root Mean Square Error = 0.006

TABLE 2

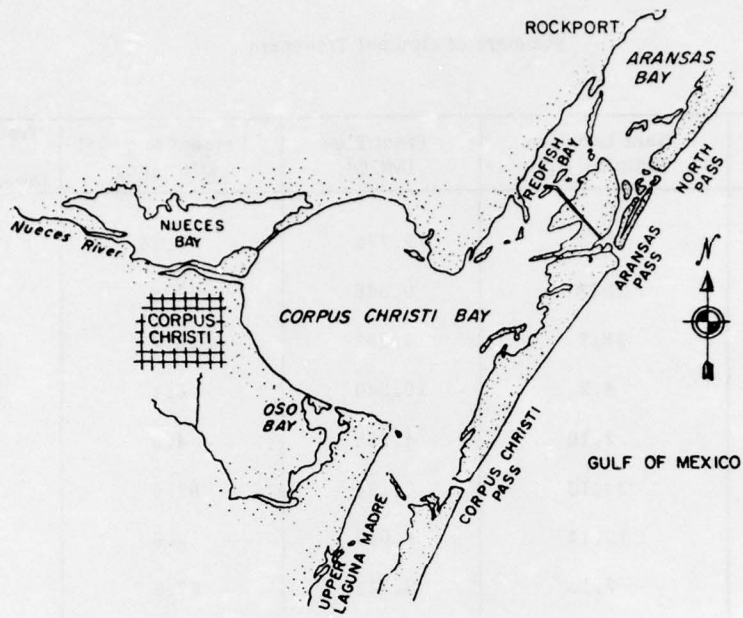
Summary of Optimal Treatment

Controllable Source No.	Plant Location Indices (i,j)	Plant Flow (MGD)	Percent Removal Efficiency	Treatment Cost in Dollars (Average, per year)
3	15,3	2.779	4.18	21,927
6	20,7	0.646	17.5	21,926
7	28,7	0.582	18.7	21,926
10	4,9	10.340	6.1	23,586
11	2,10	4.265	4.0	21,996
12	14,10	0.194	67.4	21,937
13	13,14	1.680	6.8	21,926
14	7,16	8.725	62.9	43,058
16	12,16	0.969	14.2	21,944
17	7,17	131.129	0.1	21,932
23	9,20	4.265	2.9	21,926

Total Cost = 264,084 Dollars/year

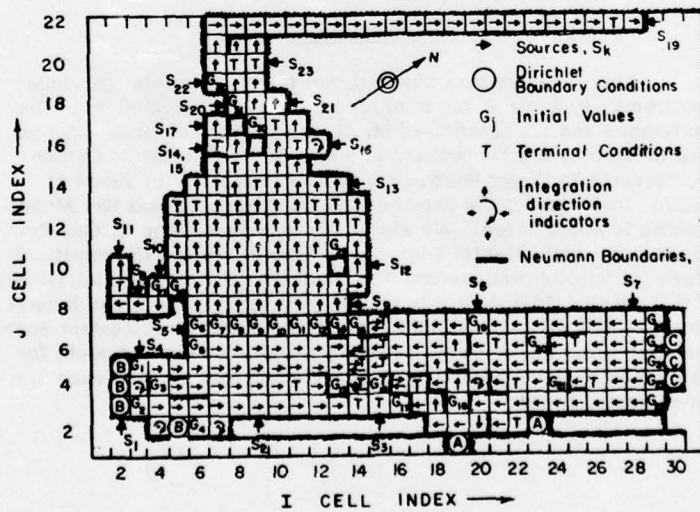
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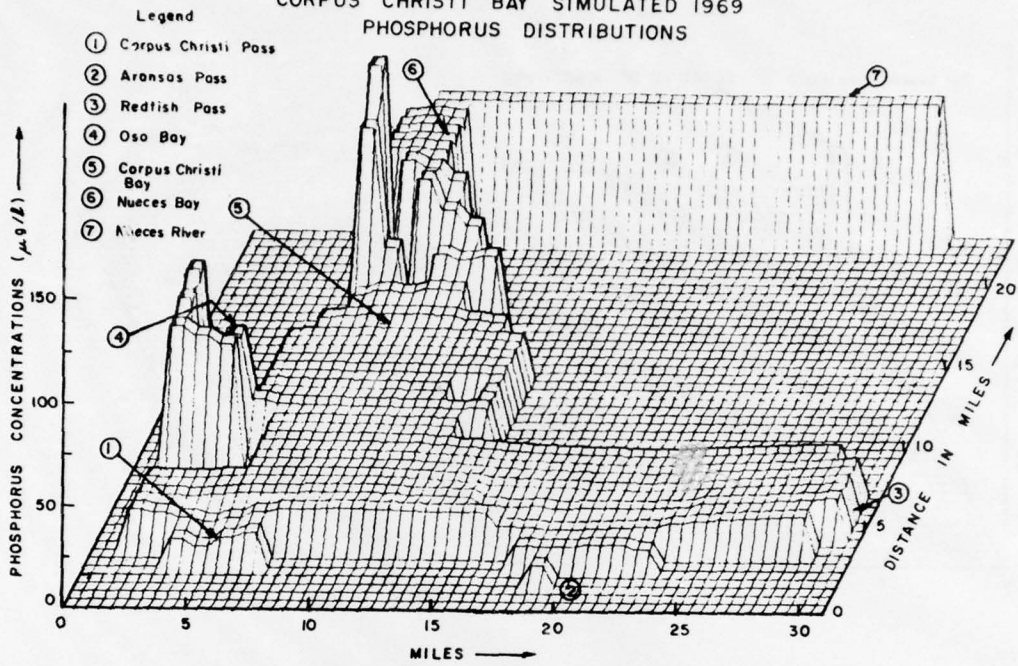
Fig. 1



COMPUTATIONAL GRID FOR MULTIPLE SHOOTING IN CORPUS CHRISTI BAY.

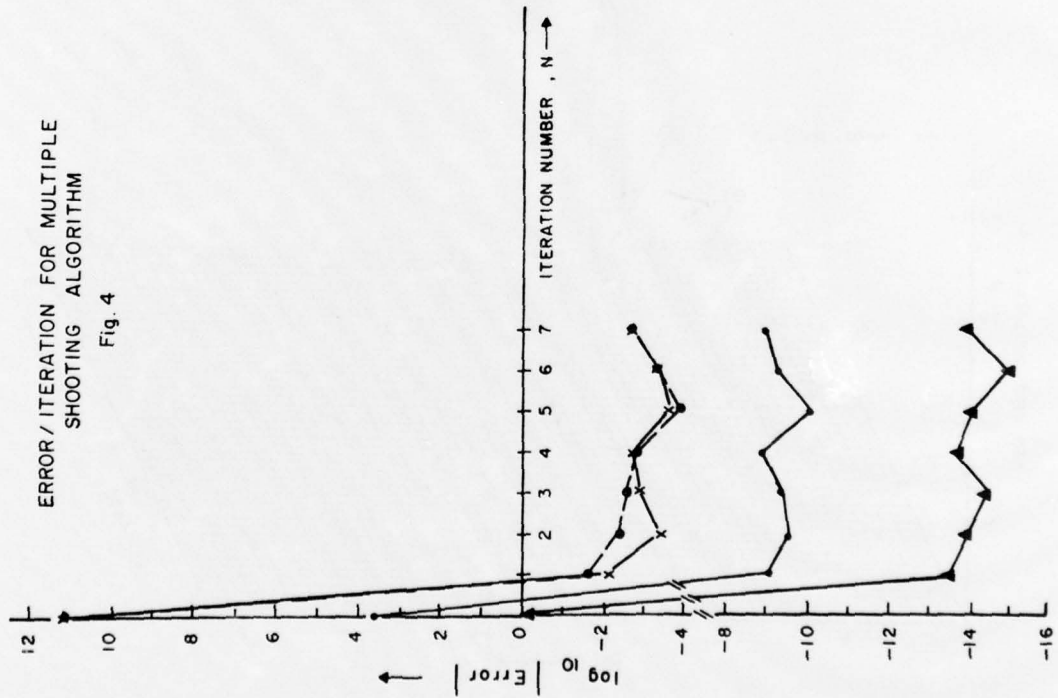
Fig. 2

Fig. 3  
CORPUS CHRISTI BAY SIMULATED 1969  
PHOSPHORUS DISTRIBUTIONS



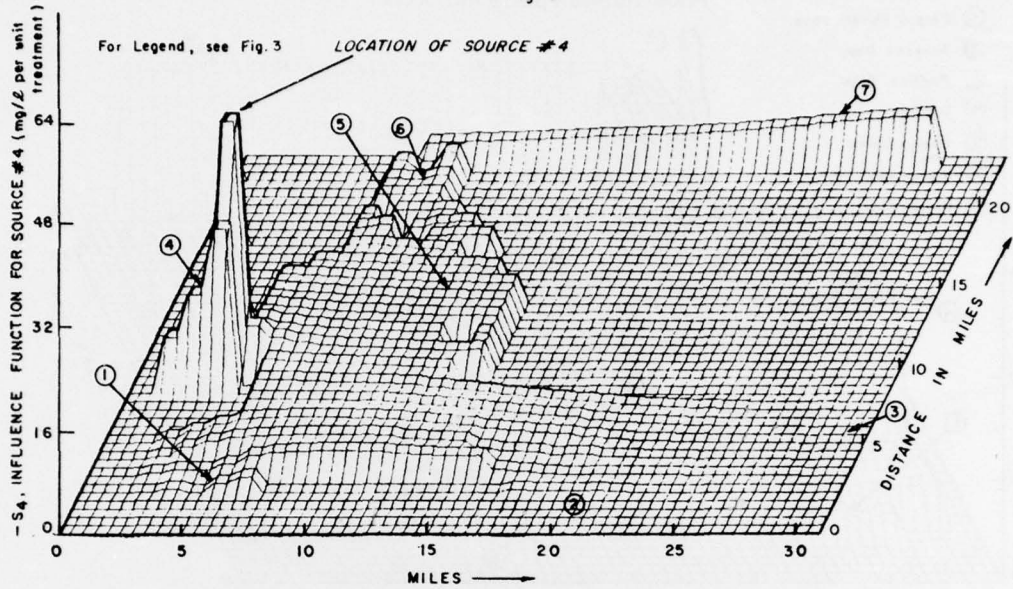
ERROR/ITERATION FOR MULTIPLE  
SHOOTING ALGORITHM

Fig. 4



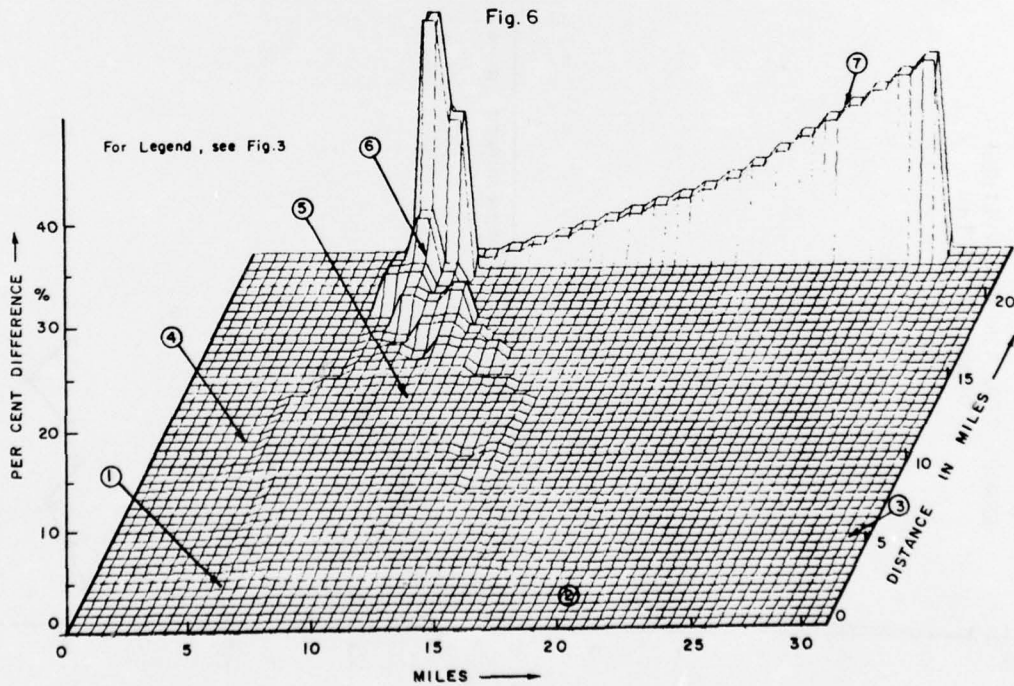
APPROXIMATE INFLUENCE FUNCTION FOR  
SOURCE NUMBER 4

Fig. 5



PER CENT DIFFERENCE BETWEEN VARIATIONAL AND SHOOTING MODELS

Fig. 6



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7. AUTHOR(s) B.J./Olufeagba, R.H./Flake and K.J./Almquist		6. PERFORMING ORG. REPORT NUMBER
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20. ABSTRACT (Continue on reverse side if necessary and identify by block number) The solution of the sparse algebraic system for a point controlled elliptic distributed parameter system by a multiple shooting and sweep algorithm is discussed. The multiple shooting and sweep algorithm enhances the convergence rate of the ordinary shooting method while achieving a significant reduction in the dimension of the linear equations to be solved. → next page (continued on back) 403789 Jmac		

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cont

The optimization algorithm for a special problem involving the minimum cost selection of source intensities with the state satisfying a specified constraint set is presented. An application of the techniques involving the analysis and management design for water quality control in Corpus Christi Bay, an estuary on the Texas Gulf Coast in the United States, is discussed. The resulting algorithm is more than twice as fast as a corresponding successive overrelaxation method.



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Fig. 7

