JOURNAL OF COMPUTATIONAL PHYSICS **114**, 280–283 (1994)

A Shooting Scheme for Boundary-Value Problems

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Received July 1, 1993; revised March 1994

A systematic shooting scheme is developed to solve a cascade of boundary value problems obtained from a small-parameter expansion of the full partial differential system. The sequence of solutions and the associated solvability conditions can be obtained simultaneously by a method without having to solve an adjoint boundary problem independently.

1. INTRODUCTION

Many vibrational problems of continuous systems and pattern-forming flows possess small parameters. In many instances the solution dependency on these parameters is desired and the perturbational technique can be employed. Some well-known examples are: the weakly nonlinear solutions slightly supercritical or subcritical of the threshold; the solutions of the onset of pattern instabilities subject to a small-amplitude parametric forcing; and the solutions of boundary value problems in the small parameters based on the normal-mode expansion from the zero-parameter solutions. In any case, if $\mathbf{L}$ represents the state operator, $\mathbf{v}$ is the solution vector, r is the control, and ε is the small parameter, then the perturbation scheme is initiated by the following expansions:

$$\begin{aligned} \mathbf{L} &= \mathbf{L}_0 + \varepsilon \mathbf{L}_1 + \varepsilon^2 \mathbf{L}_2 + \cdots, \\ \mathbf{v} &= \mathbf{v}_0 + \varepsilon \mathbf{v}_1 + \varepsilon^2 \mathbf{v}_2 + \cdots, \\ r &= r_0 + \varepsilon r_1 + \varepsilon^2 r_2 + \cdots. \end{aligned} \tag{1}$$

Each order of balance in ε yields a linear boundary value problem, and the sequence of boundary problems has to be solved in cascade. Usually, only the $O(\varepsilon^0)$ problem will be homogeneous; the higher-order problems will be inhomogeneous. The inhomogeneous terms are comprised of functions of the predecessor solutions in the sequence. The homogeneous operator in each order may or may not be the same as the operator in the lowest order. In case it is the same, a solvability condition will be required.

Traditionally, boundary value problems employing perturbational techniques for the complete solutions are very restricted. As numerical methods become widely used, computational methods permitting a systematic treatment of the problems become more useful. These methods typically have less restrictions on geometries, material properties, and the function types of the explicit solutions. This paper is to provide a generalized shooting technique in such a computational direction. The advantages of this scheme over other conventional shooting schemes are: (i) it is designed to give a convenient treatment of a sequence of boundary-value problems. The approach treats the problem as many smaller problems, thus easing the requirement for a large computer storage. In many conventional schemes, large errors may be incurred in the boundary matching conditions due to discretization errors and sensitivity of the solvability conditions, unless the step size is sufficiently small. In this scheme, the solutions appear to be less sensitive to the step size. (ii) The scheme is applicable regardless of whether the controls appear in the governing equation or in the boundary conditions. It treats different cases of combinations of homogeneous and inhomogeneous governing equation and boundary conditions. In principle, the homogeneous and inhomogeneous equations and boundary conditions can be mutually transformed. The flexibility of our scheme has rendered the need for the transformations in the pre-computing stage unnecessary. (iii) Since most systems encountered physically are nonselfadjoint, this scheme provides a simple way to treat the adjoint problem in the boundary conditions. A full independent adjoint solution analogous to the lowest order solution is not necessary.

2. THEORY

A boundary-value problem of the sequence has the following general form,

$$\mathbf{x}' = \mathbf{A}\mathbf{x} + \mathbf{f}, \tag{2}$$

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0021-9991/94 $6.00

where z is the scalar independent spatial variable, $\mathbf{A}$ is the $2n \times 2n$ (note that the number of states is even) state matrix which is, in general, z dependent; $\mathbf{x}$ is the $2n \times 1$ state vector, and $\mathbf{x}'$ is its z-derivative; and finally, $\mathbf{f}$ is the inhomogeneous term which may be dependent on the preceding solutions of the sequence. Equation (2) is subjected to boundary conditions (in general, inhomogeneous) at both ends,

$$\mathbf{Px} = \mathbf{g}, \quad \text{at} \quad z = 0, \qquad \mathbf{Qx} = \mathbf{h}, \quad \text{at} \quad z = 1, \tag{3}$$

where $\mathbf{P}$ and $\mathbf{Q}$ are constant matrices of size $n \times 2n$, each corresponding to n boundary constraints at each end; and $\mathbf{g}$ and $\mathbf{h}$ are $n \times 1$ vectors. The matrices and vectors can be complex in general. The system (2), (3) typically represents an order of the expansion in Eq. (1), where $\mathbf{A}$ and $\mathbf{x}$ represent $\mathbf{L}_k$ and $\mathbf{v}_k$ for some $k \geqslant 0$. In general, $\mathbf{L}_n$ are not equal and therefore $\mathbf{A}$ is different for each order of the expansion. For many physical problems, however, the interest is to determine the order in ε where the operator $\mathbf{L}_k$ $(k \geqslant 1)$ is equal to $\mathbf{L}_0$, implying that a solvability condition will exist. The inhomogeneous terms $\mathbf{f}$, $\mathbf{g}$, and $\mathbf{h}$ depend, again, on the predecessors $\mathbf{v}_k$.

Since the system of Eqs. (2), (3) is linear in the state, if $\mathbf{x}$ is a solution, then $\mathbf{x} + \mathbf{x}_0$ will also be a solution, where $\mathbf{x}_0$ is a scalar multiple of $\mathbf{v}_0$. Thus $\mathbf{x}_0$ satisfies the homogeneous problem,

$$\mathbf{x}' = \mathbf{Ax}; \tag{4}$$

$$\mathbf{Px} = \mathbf{0}, \quad \text{at} \quad z = 0, \qquad \mathbf{Qx} = \mathbf{0}, \quad \text{at} \quad z = 1. \tag{5}$$

The solution of the above homogeneous problem is simple by the shooting technique. The shooting technique comes from the idea that one can choose a $2n \times n$ fundamental matrix, $\mathbf{X}_0$, which contains n fundamental solutions (columns vectors) satisfying the homogenous boundary condition at the starting end, $\mathbf{PX}_0 = \mathbf{0}$. Thus the solution $\mathbf{x}_0$, is spanned by $\mathbf{X}_0$,

$$\mathbf{x}_0 = \mathbf{X}_0 \mathbf{a}_0,$$

where $\mathbf{a}_0$ is a $n \times 1$ column vector of constants. Without loss of generality, we choose $z = 0$ to be the starting end. For example, we can choose $\mathbf{X}_0(0)$ to be in the form of

$$\mathbf{X}_0(0) = \begin{bmatrix} -\mathbf{P}_1^{-1}\mathbf{P}_2 \\ \mathbf{I}_n \end{bmatrix},$$

where $\mathbf{P} = [\mathbf{P}_1 \mid \mathbf{P}_2]$ such that $\mathbf{P}_1$ is non-singular. At the matching end, $z = 1$, the boundary condition requires

$$(\mathbf{QX}_0)\, \mathbf{a}_0 = \mathbf{0}. \tag{6}$$

For non-trivial $\mathbf{a}_0$, we require

$$\det[\mathbf{QX}_0] = \mathbf{0}. \tag{7}$$

The condition above places a constraint of the parameter set. Therefore, solutions can only exist on a hyperspace of a lower dimension of the parameter space. In general, an iterative method has to be used to compute the parameters of non-trivial solutions.

With the inhomogeneous terms in Eqs. (2), (3), a solution may or may not exist, since now these inhomogeneous terms cannot be arbitrary. They are constrained not entirely separately, but together by a solvability condition (a result known as the Fredholm's alternative) instead, in order to preserve consistency. Since the inhomogeneous terms depend on the lower order solutions, the solvability condition therefore serves to determine the subsequent terms in the expansion in a unique fashion. More conventionally, the solvability conditions can be obtained by a projection of the equation space onto the adjoint solution space. First, one has to solve an adjoint problem like the homogeneous problem. Then, one has to perform an averaging. The job can be quite tedious. Consider, for example, a more restrictive case corresponding to $\mathbf{f} \neq \mathbf{0}$ and $\mathbf{g} = \mathbf{0}$ and $\mathbf{h} = \mathbf{0}$. The adjoint problem can be defined as

$$\tilde{\mathbf{x}}' = -\mathbf{A}^{+}\tilde{\mathbf{x}}, \tag{8}$$

where the superscript "+" denotes the adjoint operator (transpose and complex conjugate). The problem is then subject to boundary conditions

$$\tilde{\mathbf{P}}\tilde{\mathbf{x}} = \mathbf{0}, \quad \text{at} \quad z = 0, \qquad \tilde{\mathbf{Q}}\tilde{\mathbf{x}} = \mathbf{0}, \quad \text{at} \quad z = 1, \tag{9}$$

where the boundary matrices are chosen so that $\tilde{\mathbf{x}}$ satisfies

$$\mathbf{x}_0^+(0)\, \tilde{\mathbf{x}}(0) = \mathbf{x}_0^+(1)\, \tilde{\mathbf{x}}(1). \tag{10}$$

In autonomous problems, $\mathbf{x}_0^+(0)\, \tilde{\mathbf{x}}(0) = 0$ also implies that $\mathbf{x}_0^+(1)\, \tilde{\mathbf{x}}(1) = 0$; thus one simply defines $\tilde{\mathbf{x}}(0)$ such that $\mathbf{x}_0^+(0)\, \tilde{\mathbf{x}}(0) = 0$; $\tilde{\mathbf{P}}$ is defined accordingly so that $\tilde{\mathbf{P}}\tilde{\mathbf{x}}(0) = \mathbf{0}$. For non-autonomous problems, the selection of $\tilde{\mathbf{P}}$ and $\tilde{\mathbf{Q}}$ may involve some intelligent judgements. But, in general, there are numerous ways to define the adjoint problem in this manner. Once $\tilde{\mathbf{x}}$ is found, the solvability condition is given by

$$\int_0^1 \tilde{\mathbf{x}}^{+}\mathbf{f}\, dz = 0. \tag{11}$$

Although the method is in principle valid, there may be practical problems. If the projection for the particular choice of $\tilde{\mathbf{x}}$ is weak, then Eq. (11) can incur large errors, especially for large n, due to the summation of many entries in the vectors which in general have large variations of magnitude. As this type of boundary-value problem seems quite elementary, little attention has been focused on an improved method to solve the problem. Here, we show that with our shooting technique, a simultaneous treatment of both the solution and the solvability condition becomes possible, by splitting the general solution into the sum of a particular solution and a homogeneous solution. For an order when $\mathbf{L}_k$ is different from $\mathbf{L}_0$, no solvability condition exists. The homogeneous solution is employed to satisfy the boundary conditions while the particular solution is employed to satisfy the governing equation. For an order when $\mathbf{L}_k$ equals $\mathbf{L}_0$, an additional solvability condition will be sought. Since the inhomogeneous forcing may have secular contributions, the trick here is to use the fundamental set of the zeroth order solution to span the current order's homogeneous solution. The solvability condition is then determined on the level of the boundary conditions. No additional integration such as those of Eq. (11) will be required.

Following this idea we let the solution of Eqs. (2, 3), $\mathbf{x}$, be split, such that

$$\mathbf{x} = \mathbf{X}_h \mathbf{a}_h + \mathbf{x}_p. \tag{12}$$

The particular solution $\mathbf{x}_p$ satisfies

$$\mathbf{P}\mathbf{x}_p(0) = \mathbf{g}.$$

Given $\mathbf{P}$ and $\mathbf{g}$, $\mathbf{x}_p(0)$ can be solved. If $\mathbf{P}$ contains the control of the problem, then the condition above will only provide a guess, which has to be improved iteratively. We now integrate $\mathbf{x}_p$ forward according to

$$\mathbf{x}_p' = \mathbf{A}\mathbf{x}_p + \mathbf{f},$$

from $z=0$ to $z=1$. At $z=1$, the coefficients $\mathbf{a}_h$ are now determined from

$$(\mathbf{Q}\mathbf{X}_h)\,\mathbf{a}_h = (\mathbf{h} - \mathbf{Q}\mathbf{x}_p). \tag{13}$$

The above equation can be inverted to give $\mathbf{a}_h$. In the case when $\mathbf{X}_h$ is equal to $\mathbf{X}_0$, then the system is self-consistent, provided

$$\tilde{\mathbf{a}}^{+}(\mathbf{h} - \mathbf{Q}\mathbf{x}_p) = 0, \tag{14}$$

where $\tilde{\mathbf{a}}$ satisfies

$$(\mathbf{X}_0^{+}\mathbf{Q}^{+})\,\tilde{\mathbf{a}} = \mathbf{0}. \tag{15}$$

Now $\tilde{\mathbf{a}}$ is the adjoint of $\mathbf{a}_0$. Equation (14) is the solvability condition in a boundary form. If the control parameter occurs in the starting boundary or in both boundaries, then the solvability condition can only be solved iteratively.

Consider the previous case again, where $\mathbf{f} \neq \mathbf{0}$ but $\mathbf{g} = \mathbf{0}$ and $\mathbf{h} = \mathbf{0}$. Suppose $\mathbf{f} = \mathbf{f}_1 + R\mathbf{f}_2$, where R is the control. Now let $\mathbf{x}_p = \mathbf{x}_{p1} + \mathbf{x}_{p2}$. The latter satisfies

$$\mathbf{x}_{p1}' = \mathbf{A}\mathbf{x}_{p1} + \mathbf{f}_1, \qquad \mathbf{x}_{p2}' = \mathbf{A}\mathbf{x}_{p2} + \mathbf{f}_2.$$

Then from Eq. (14), R is determined by

$$R = -\frac{\tilde{\mathbf{a}}^{+}(\mathbf{h} - \mathbf{Q}\mathbf{x}_{p1})}{\tilde{\mathbf{a}}^{+}\mathbf{Q}\mathbf{x}_{p2}}. \tag{16}$$

3. EXAMPLES

The shooting scheme has been used in computing solutions of the problem of delayed onset in convection of a plane layer of fluid, subjected to small oscillations in the wall. A sample of examples will be briefly discussed here.

i. *The Rayleigh–Bénard Convection*

For Rayleigh–Bénard convection [1], the control is the supercritical increment of the Rayleigh number in the governing equation. For Marangoni convection [2], the control is the increment of Marangoni number that appears in one of the free surface conditions. When both buoyancy and surface tension effects are allowed simultaneously, we have both controls. We refer readers to the references for the details of the problems. Here we provide only some computational results of these problems to illustrate the use of the scheme. Consider the problem of [1], where the upper plate of the layer is held fixed. In [1, Fig. 1], the family of curves (i), (ii), and (iv) show the onset curves of the control parameter R/Pr^2 versus the modulation frequency $\beta^2\,\mathrm{Pr}$ for Prandtl numbers Pr equal to 0.5, 1.0, and 10.0, respectively. These curves were obtained by explicit integration of their

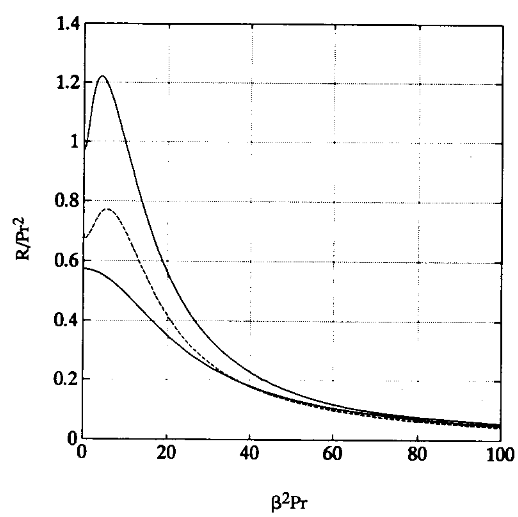

FIGURE 1

Eqs. (3.11) and (3.12). Here we reproduce the set of curves using our shooting scheme, Eqs. (12)–(16). We use a 20-step integration, which is significantly less than that used in [1]. In Fig. 1, the higher solid, middle dashed, and lower solid lines correspond to Pr = 0.5, 1.0, and 10.0, respectively.

ii. *The Marangoni and Rayleigh–Bénard Convection*

Since Rayleigh–Bénard convection does not involve inhomogeneous terms in the boundary conditions, the flexibility of our shooting scheme has not been fully demonstrated. In a recent paper, we study the delayed onset of the mixed Marangoni and Rayleigh–Bénard convection [2] and use the scheme for the computations. The boundary conditions involve a deformable surface and are significantly more complex [2]. Consider

$$\mathbf{x}' = \mathbf{A}\mathbf{x} + \mathbf{f}_1 + R\mathbf{f}_2 \tag{17}$$

subject to

$$\mathbf{Q}\mathbf{x} = \mathbf{0}, \quad \text{at} \quad z = 1,$$
$$\mathbf{P}\mathbf{x} = \mathbf{h}_1 + M\mathbf{h}_2, \quad \text{at} \quad z = 0.$$

where $\mathbf{x}$ is the state vector; $\mathbf{f}_j$ and $\mathbf{h}_j$, $j = 1, 2$, are known vector functions. Now in addition to the control R, M represents the supercritical increment in the Marangoni

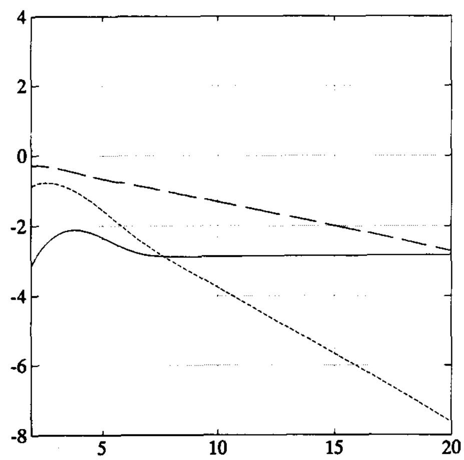

FIGURE 2

number. The single solvability condition governing these two controls is given by

$$M - bR = c; \tag{18}$$

where b and c are defined as

$$b = \frac{(\tilde{\mathbf{a}}^+\mathbf{P}\mathbf{x}_{p2})}{(\tilde{\mathbf{a}}^+\mathbf{h}_2)}, \qquad c = \frac{\tilde{\mathbf{a}}^+(\mathbf{P}\mathbf{x}_{p1} - \mathbf{h}_1)}{(\tilde{\mathbf{a}}^+\mathbf{h}_2)}.$$

The vector $\tilde{\mathbf{a}}$ satisfies $(\mathbf{X}_0^+\mathbf{P}^+)\,\tilde{\mathbf{a}} = \mathbf{0}$; $\mathbf{X}_0$ is a matrix of the column vectors which form half of the fundamental set of the homogeneous system satisfying the wall condition $\mathbf{Q}\mathbf{x} = \mathbf{0}$ at $z = 1$; and finally $\mathbf{x}_{pj}$, $j = 1, 2$, satisfy, respectively,

$$\mathbf{x}' = \mathbf{A}\mathbf{x} + \mathbf{f}_j, \qquad j = 1, 2,$$

with $\mathbf{x}_{pj} = \mathbf{0}$ at $z = 1$. In Fig. 2, we show a sweep of the coefficients b (solid) and c (dashed) of the solvability condition. Also shown is the value of $-c/b$ (long-dashed). The horizontal axis presents the Prandtl number. The other parameters of the example correspond to a long-wavelength regime of the convection: $\beta = 1.2$, $k = 0.1$, $\chi = 3.4$, and Bo = 0.067, where k is the wavenumber, χ is the Galileo number, and Bo is the Bond number.

4. REMARKS

The shooting scheme provided here is simple and easy to implement numerically. It permits an efficient means for solving the sequence of boundary problems, where the state matrix can be non-self-adjoint and the boundary conditions can be inhomogeneous and non-symmetric. Multiple control parameters are permitted and they can occur in the governing equation or in the boundary conditions. The scheme is less sensitive to boundary errors. Thus it reduces the need for very fine-step integrations.

ACKNOWLEDGMENTS

This work was supported by NASA Grant NAG3-1456. I thank Professor R. E. Kelly for numerous stimulating discussions.

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