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On Domain Decomposition and Shooting Methods for Two-Point Boundary Value Problems

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ABSTRACT. The fundamental properties of a shooting method for two-point boundary value problems are examined and its relation to a nonoverlapped domain decomposition technique is discussed. We address and tackle the instability problem. We extend the nonoverlapped domain decomposition to multisubdomain cases and derive an efficient parallel shooting algorithm. Numerical examples include linear problems in convection-diffusion and nonlinear problems in semiconductor device modelling.

1. Introduction

This paper intends to review some of the fundamental properties of a shooting method for two-point boundary value problems and the connection of these properties to domain decomposition methods. Idea related to this subject can be found in [5] [6]. Similar approach for two-point boundary value problems was reported in [4]. Attention is restricted to the following class of second order ordinary differential equations

$$\frac{d^2\phi}{dx^2} + Q(x,\phi,\frac{d\phi}{dx}) = 0 \in \Omega = \{x : a < x < b\}, \tag{1}$$

subject to boundary conditions of either

$$\phi(a) = \phi_a , \frac{d\phi(b)}{dx} = \phi'_b , \tag{2}$$

or

$$\phi(a) = \phi_a , \phi(b) = \phi_b , \tag{3}$$

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where ϕ_a, ϕ'_b and ϕ_b are given constants. Assume that the function $Q(x, \phi, d\phi/dx)$ is continuous and is Lipschitz bounded so that unique solution of (1) exists for each of the above two types of boundary conditions.

2. Elementary Properties of a Shooting Method

A shooting method for (1) subject to boundary conditions (2) can be obtained by choosing a trial value λ_a and then by solving the initial value problem

$$\frac{d^2u}{dx^2} = -Q(x, u, \frac{du}{dx}) , \; u(a) = \phi_a , \; u'(a) = \lambda_a . \tag{4}$$

We assume that the solution $u(x;\lambda)$ of (4) does not suffer from any instability. A family of solutions $F\{u(x;\lambda)\}$ is obtained subject to the variation of the parameter λ_a. This parameter is adjusted and the initial value problem (4) is solved with the adjusted λ_a until the derivative of the solution of (4) at $x = b$ is sufficiently close to ϕ'_b. It is clear at this stage that finding the correct value of λ_a is equivalent to finding a root of the nonlinear function [1] [3],

$$f(\lambda_a) \equiv \frac{\partial u(b;\lambda_a)}{\partial x} - \phi'_b = 0 . \tag{5}$$

To approximate the root of $f(\lambda_a) = 0$, we write the equation as

$$\lambda_a = G(\lambda_a) \equiv \lambda_a - \alpha f(\lambda_a) , \tag{6}$$

and consider the fixed point iteration scheme

$$\lambda_a^{(n+1)} = \lambda_a^{(n)} - \alpha f(\lambda_a^{(n)}) , \; n = 0, 1, 2, \ldots . \tag{7}$$

Assuming G satisfies a Lipschitz condition on λ_a and that a suitable choice of α is being used so that the sequence $\{\lambda_a^{(n)}\}$ is a converging sequence which converges to a root of (5). A treatise on the choice of α can be found in [1] [2].

One disadvantage of the above shooting method lies in the fact that an initial value problem has to be solved at each step of the iteration scheme (7). The flexibility of using parallel architecture is very restricted because of the nature of the initial value problem. Since the initial value problem (4) has a unique solution for each value of λ_a and if the iteration scheme (7) converges to a root of (5), then at each step of the iteration there exists a one-to-one correspondence between $\lambda_a^{(n)}$ and $\lambda_b^{(n)} \equiv u(b;\lambda_a^{(n)})$. Hence we have,

PROPOSITION 1. *For any converging sequence $\{\lambda_a^{(n)}\}$ which converges to a root of the nonlinear equation $f(\lambda_a) \equiv \frac{\partial u(b;\lambda_a)}{\partial x} - \phi'_b = 0$ such that $u(x;\lambda_a^{(n)})$ is the solution of the intial value problem,*

$$\frac{d^2u}{dx^2} = -Q(x, u, \frac{du}{dx}) , \; u(a) = \phi_a , \; u'_a(a) = \lambda_a^{(n)} , \tag{8}$$

there exists a corresponding converging sequence $\{\lambda_b^{(n)} = u(b; \lambda_a^{(n)})\}$ *such that the solution* $v(x; \lambda_b^{(n)})$ *of the boundary value problem*

$$\frac{d^2v}{dx^2} + Q(x, v, \frac{dv}{dx}) = 0 \,,\; v(a) = \phi_a \,,\; v(b) = \lambda_b^{(n)} \,, \tag{9}$$

is equal to the solution $u(x; \lambda_a^{(n)})$ *of the initial value problem.*

COROLLARY. *For any converging sequence* $\{\lambda_b^{(n)} := \lambda_b^{(n)} - \beta g(\lambda_b^{(n-1)})\}$ *which converges to a root of the nonlinear equation* $g(\lambda_b) \equiv \frac{\partial v(b;\lambda_b)}{\partial x} - \phi'_b = 0$ *where* $v(x; \lambda_b^{(n)})$ *is the solution of* (9), *then there exists an* $\alpha = \alpha(\beta)$ *such that the solution of the boundary value problem* (9) *is equal to the solution of the initial value problem* (8) *with* $\lambda_a^{(n)} = \frac{\partial v(a;\lambda_b^{(n)})}{\partial x}$.

EXAMPLE 1. The initial value problem

$$\frac{d^2u}{dx^2} = \gamma\frac{du}{dx} \,,\; u(a) = \phi_a \,,\; u'(a) = \lambda_a^{(n)} \,,$$

has solution

$$u(x; \lambda_a^{(n)}) = \phi_a + \frac{\lambda_a^{(n)}}{\gamma}(\frac{e^{\gamma x} - e^{\gamma a}}{e^{\gamma a}}) \,.$$

The boundary value problem

$$\frac{d^2v}{dx^2} - \gamma\frac{dv}{dx} = 0 \,,\; v(a) = \phi_a \,,\; v(b) = \lambda_b^{(n)} \,,$$

has solution

$$v(x; \lambda_b^{(n)}) = \phi_a + \frac{\lambda_b^{(n)} - \phi_a}{e^{\gamma b} - e^{\gamma a}}(e^{\gamma x} - e^{\gamma a}) \,.$$

Substituting $\lambda_a^{(n)} = \frac{\partial v(a;\lambda_b^{(n)})}{\partial x}$ into the expression for $u(x; \lambda_a^{(n)})$, we obtain $v(x) = u(x)$. From the expression $\lambda_b^{(n+1)} = \lambda_b^{(n)} - \beta g(\lambda_b^{(n)})$, we can deduce that $\lambda_a^{(n+1)} = \lambda_a^{(n)} - \alpha f(\lambda_a^{(n)})$, where $\alpha = \beta\frac{\gamma e^{\gamma a}}{e^{\gamma b} - e^{\gamma a}}$.

Since the stability of (9) is easier to control than that of (8) therefore it seems better to work with (9). It follows from the Corollary that we can establish a variant of the above shooting method as following,

PROPOSITION 2. *The solution of* (1) *subject to boundary conditions* (2) *can be obtained by finding a root of the nonlinear function* $g(\lambda) \equiv \frac{\partial v(b;\lambda_b)}{\partial x} - \phi'_b = 0$, *where* $v(x; \lambda_b)$ *is the solution of the boundary value problem*

$$\frac{d^2v}{dx^2} + Q(x, v, \frac{dv}{dx}) = 0 \,,\; v(a) = \phi_a \,,\; v(b) = \lambda_b \,. \tag{10}$$

Proposition 2 complicates the solution process of (1), but is used in the context of a domain decomposition. The advantage of the present variant is that (10) involves solutions of boundary value problems and the instability introduced by initial value problems can be eliminated.

3. A Nonoverlapped Domain Decomposition Method

For simplicity, the following two-point boundary value problem is considered,

$$\frac{d^2\phi}{dx^2} + Q(x, \phi, \frac{d\phi}{dx}) = 0 \in \Omega = \{x : a < x < c\}, \tag{11}$$

subject to Dirichlet boundary conditions $\phi(a) = \phi_a$ and $\phi(c) = \phi_c$. We construct two nonoverlapped subdomains $\Omega_1 = \{x : a < x < b\}$ and $\Omega_2 = \{x : b < x < c\}$ and the interface of Ω_1 and Ω_2 is $\Gamma_{12} = \{x : x = b\}$. For the problem given by (11), the coupling at the interface Γ_{12} is well known to be (a) the continuity of the function and (b) the continuity of the derivative of the function at that point.

It is obvious that one can use Proposition 2 to solve the two subproblems provided we know the value of ϕ'_b. The situation now is analogous to a shooting exercise in which we require the two shells fired from two artillery men based at $x = a$ and $x = c$ to collide at the interface Γ_{12}. We can interpret the above coupling conditions as the height and the slope of the trajectory at the point of collision. Application of Proposition 2 is achieved by simply reducing the number of variational parameters to one, in which case we have a one parameter nonlinear equation of which the solution is required. This discussion is summarised in the following Proposition.

PROPOSITION 3. *The boundary value problem* (11) *is replaced by the following two subproblems,*

$$\frac{d^2u_1}{dx^2} + Q(x, u_1, \frac{du_1}{dx}) = 0 \in \Omega_1, \; u_1(a) = \phi(a), \; u_1(b) = \lambda, \tag{12}$$

and

$$\frac{d^2u_2}{dx^2} + Q(x, u_2, \frac{du_2}{dx}) = 0 \in \Omega_2, \; u_2(b) = \lambda, \; u_2(c) = \phi(c), \tag{13}$$

and the nonlinear function

$$D(\lambda) \equiv \frac{\partial u_1(b;\lambda)}{\partial x} - \frac{\partial u_2(b;\lambda)}{\partial x} = 0. \tag{14}$$

The two subproblems together with the nonlinear function is a variant of shooting method where the matching is chosen at $x = b$.

One advantage of the current method compared with the previous shooting method is that the two subproblems can be decomposed and indepently computed, thus ensuring intrinsic parallelism. The other advantage is that the subproblems are now boundary value problems which can avoid instability caused by solving initial value problems. Furthermore each of the subproblems is smaller than the original problem and is easier to solve. In order to solve (14), we use the fixed point iteration scheme, $\lambda^{(n+1)} = \lambda^{(n)} - \alpha_n D(\lambda^{(n)})$, where $\alpha_n := \alpha_{n-1}|D(\lambda^{(n-1)})|/|D(\lambda^{(n)}) - D(\lambda^{(n-1)})|$, details of which can be found in [6].

EXAMPLE 2. Consider $\frac{d^2\phi}{dx^2} - \gamma\frac{d\phi}{dx} = 0$, subject to $\phi(0) = 0$, $\phi(1) = 1$. Here $\gamma \gg 1$ and $b = 1 - \frac{1}{\gamma}$, "exact subsolver" means an analytic solution is obtained in the corresponding subdomain, and h is the mesh size in a finite difference scheme. In the case of finite difference method, we use the same h in both of the subdomains.

γ	n	$\lambda^{(n)}$	$\phi(b)$	$\lvert\phi(b) - \lambda^{(n)}\rvert$
10	2	0.36785	0.36785	0.37×10^{-7}
30	2	0.36788	0.36788	0.81×10^{-7}
50	2	0.36788	0.36788	0.37×10^{-6}

Table 1 : Convergence results using an exact solver.

h	n	$\lambda^{(n)}$	$\lvert\phi(b) - \lambda^{(n)}\rvert$
0.02	3	0.36663	0.12×10^{-2}
0.01	3	0.36754	0.31×10^{-3}
0.005	3	0.36777	076×10^{-4}
0.0025	3	0.36783	0.17×10^{-4}

Table 2: Convergence results for $\gamma = 10$ using a 2nd order difference scheme.

4. A Multiple Shooting Method

If the process in Proposition 3 is carried out recursively for every subsequent subdomain, then we have $\Omega_k = \{x : b_{k-1} < x < b_k\}$, $k = 1, 2, \dots, s+1$, where $b_0 = a$ and $b_{s+1} = c$. Here Ω_k's denote a set of non-overlapped subdomains. The interfaces are located at $x = b_k$, $k = 1, 2, \dots, s$ where the solutions at these interfaces are required. Since each pair of neighbouring subdomains is exactly the same as that given by Proposition 2, the multi-subdomain case derived from the above discussion can be considered as a multiple shooting technique.

PROPOSITION 4. *The boundary value problem given by* (11) *is replaced by the following* $s+1$ *subproblems,*

$$(15)\quad \frac{d^2u_k}{dx^2} + Q(x, u_k, \frac{du_k}{dx}) = 0 \in \Omega_k\ ,\ u_k(b_{k-1}) = \lambda_{k-1}\ ,\ u_k(b_k) = \lambda_k\ ,$$

for $k = 1, 2, \dots, s+1$, *with* $u_1(a) = \phi(a)$ *and* $u_{s+1}(c) = \phi(c)$, *and the nonlinear vector function*

$$(16)\qquad D(\lambda) = [D_k(\lambda)] \equiv [\frac{\partial u_k(b_k;\lambda)}{\partial x} - \frac{\partial u_{k+1}(b_k;\lambda)}{\partial x}] = 0$$

where $\lambda = [\lambda_1\ \lambda_2\ \dots\lambda_s]$ *is an* s*-vector. These subproblems together with the nonlinear vector function is a multiple shooting algorithm where the matching is done at the interfaces.*

In order to solve $D(\lambda) = 0$, a fixed point iteration scheme similar to that given above is used. Here α_n can be chosen either as the matrix $[J(\lambda^{(0)})]^{-1}$

where $J(\lambda^{(0)}) = D'(\lambda^{(0)})$ which reduces the scheme to Newton's iteration, or as a scalar adaptive parameter given by

$$\alpha_n := \alpha_{n-1} \frac{\| D(\lambda^{(n-1)}) \|_2}{\| D(\lambda^{(n)}) - D(\lambda^{(n-1)}) \|_2} \tag{17}$$

Details of the choices can be found in [6].

EXAMPLE 3. We solve the same problem as that given by Example 2 using an analytic subproblem solver and present the number of iterations, n, required to update the interfaces which are evenly distributed across the physical domain.

$s \setminus \gamma$	10	20	30	40	50
3	14	15	15	13	11
7	23	21	18	20	20
15	37	35	34	37	31
31	96	62	58	51	52

Table 3: Convergence results using α_n defined in (17).

First, we construct the Jacobian matrix $J(\lambda^{(0)})$ which requires $2s$ subproblem solves. Each iteration involves $s + 1$ subproblem solves in order to compute $D(\lambda^{(n)})$. By taking $\alpha_n = [J(\lambda^{(0)})]^{-1}$, we require $n = 2$ iterations to update the interfaces. We achieve an efficient multiple shooting algorithm in a coarse-grain parallel computing environment provided we can invert $J(\lambda^{(0)})$ efficiently. Second, we use the scalar adaptive α_n in (17) and record n in Table 3. Here we do not invert $J(\lambda^{(0)})$ but the penalty is an increase in n. However the simple communication which involves only exchanging neighbouring information provides another efficient multiple shooting algorithm in a coarse-grain parallel computing environment. We observe that the number of iterations n is independent of the problem type, but increases as the number of interfaces s increases.

EXAMPLE 4. A nonlinear electrostatic problem [7] in normalised variables is tested. The problem is described by (11) with $a = 0$ and $c = 180$ and is subjected to boundary conditions $\phi(0) = 0$ and $\phi(180) = 10$. The function Q is given as

$$Q = \Gamma(x) + e^{(\phi_+ - \phi)} - e^{(\phi - \phi_-)} .$$

Here

$$\Gamma = -Ne^{-x^2/e^2} + Ne^{-(c-x)^2/e^2} , \; N = \frac{1480}{1 - e^{-1}} ,$$

$$\phi_+ = \phi(a) + \ln \left\{ -\frac{\Gamma(a)}{2} + \sqrt{\left(\frac{\Gamma(a)}{2}\right)^2 + 1} \right\} ,$$

$$\phi_- = \phi(c) - \ln \left\{ \frac{\Gamma(c)}{2} + \sqrt{\left(\frac{\Gamma(c)}{2}\right)^2 + 1} \right\} ,$$

We evenly distribute the interfaces across the entire domain, and we use equal meshes and a second order difference scheme throughout the subdomains. We use the adaptive α_n as that given above. Table 4 records the number of iteration, n, required to update the interfaces.

$s \setminus h$	2	1	0.5	0.25	0.125
2	8	8	7	8	8
4	15	15	14	14	12
8	29	30	24	24	20
14	358	124	100	81	75

Table 4: Convergence results for the nonlinear electrostatic problem.

Note that the number of iterations n is independent of the mesh size h, but is dependent of the number of interfaces s. It is also observed that $n \approx 3s$ for small values of s and that n becomes unreasonably large for large values of s.

5. Conclusion

A framework for domain decomposition methods is built on the properties of a shooting method. A two subdomain case was presented and the convergence results are the same as the shooting method. The two subdomain case is extended to the multi-subdomain case. The multi-subdomain case provides an efficient multiple shooting algorithm on coarse-grain parallel architectures. Linear and nonlinear examples are included.

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