JOURNAL OF COMPUTATIONAL PHYSICS 119, 132–141 (1995)

Adaptive Pseudo-Spectral Domain Decomposition and the Approximation of Multiple Layers*

ALVIN BAYLISS, MARC GARBEY† AND BERNARD J. MATKOWSKY

Department of Engineering Sciences and Applied Mathematics, Northwestern University, Evanston, Illinois 60208

Received December 9, 1993; revised November 28, 1994

When Chebyshev pseudo-spectral methods are used with domain decomposition procedures in the numerical solution of partial differential equations, the use of multiple domains can significantly affect the accuracy of the approximation. This is particularly true when the solution exhibits layer type behavior, i.e., there are narrow regions of rapid variation. Accuracy may be enhanced if the interfaces between adjacent subdomains are such that large gradients occur near the interfaces, while accuracy can be degraded if the rapid variations occur in the interior of the subdomains. The use of appropriate mappings within each subdomain can improve the accuracy of the approximation by choosing mappings so that the transformed function is more readily approximated by a low order polynomial. The particular choice of mappings, however, depends critically on whether the solution exhibits boundary layer or interior layer behavior within each subdomain. We analyze the relationship between interface location and mappings required to obtain an efficient approximation of such functions. We compare two strategies, both based on constructing subdomains so that each subdomain contains only one layer. In the first strategy interface locations are chosen so that the rapid variations occur as interior layers and mappings are employed which enhance the resolution of such layers (strategy I for interior). In the second strategy interface locations are chosen so that rapid variations occur as boundary layers and mappings are employed which enhance resolution of boundary layers (strategy B for boundary). Both strategies lead to adaptive domain decomposition procedures based entirely on the locations of the layers. We demonstrate that strategy B offers superior accuracy for a given computational effort and employ this strategy in developing an adaptive domain decomposition method for problems with multiple layers. Both strategies are comparable regarding spectral radii of the resulting matrices, and we conclude that domain decomposition itself cannot result in larger stable time steps when accuracy of the approximation of the layer is considered. The adaptive domain decomposition method is illustrated by the computation of both axisymmetric and cellular flames with a sequential reaction mechanism involving two reaction zones.

* Supported in part by NSF Grants MMS 91-02981 and 93-01635, DOE Grant DEFG02ER25027 and a NATO Collaborative Research Grant.

† Permanent address: Laboratoire D'analyse Numerique, URA 740, Université Lyon 1, Lyon, France.

1. INTRODUCTION

The accuracy of Chebyshev pseudo-spectral methods in approximating solutions to partial differential equations can be significantly degraded when used to approximate solutions which have localized regions of rapid variation (layers). Such problems occur in many areas of application, such as combustion, fluid dynamics, solidification, solid mechanics, and wave propagation, to name but a few. The approximations may exhibit spurious oscillations which can lead to nonlinear instabilities or spurious predictions of solution behavior. Accuracy is also sensitive to the locations of the regions of rapid variation. For example, there is significant evidence that pseudo-spectral methods are more effective in approximating functions where rapid variations or large gradients occur close to the boundary of the domain, as opposed to its interior, e.g., [7, 28].

The problem of computing a single layer can be handled by employing suitably chosen mappings so that in the mapped coordinate the solution varies gradually and can thus be well approximated by a low-order polynomial. A family of mappings, suitable primarily for internal layers, was introduced in [7] and was compared with other families of mappings, in particular mappings suitable to enhance the resolution of boundary layers. Such families of mappings form the basis of an adaptive pseudo-spectral method which has been used to accurately solve a range of problems involving solutions with localized regions of rapid variation (e.g., [1, 4–6, 18]).

In this method mappings are chosen adaptively from a prescribed family of mappings so as to minimize a functional of the solution which measures the error in the approximation. This method allows the benefits of spectral and pseudo-spectral methods, e.g., high accuracy, to be realized for the approximation of rapidly varying functions without the spurious oscillations which often accompany the use of spectral methods in approximating such functions. To date, both the proposed families of mappings and the computations have been primarily for problems involving either only one region of rapid variation or several closely spaced regions which are effectively treated as a single region.

0021-9991/95 $6.00

The problem of resolving functions with localized regions of rapid variation is particularly important in combustion. Activation energies of the chemical reactions in combustion are typically large. As a result the reaction terms are significant only in narrow regions termed reaction zones. In the limit of infinite activation energy reaction zones shrink to surfaces termed flamed fronts, across which certain jump conditions hold. While the flame front model is well suited for mathematical analysis (e.g., [23, 24]), numerical computations are generally conducted for the case of finite activation energy, where the flame occupies a region of small but finite thickness. In this case the solution is a smooth, infinitely differentiable function, with large gradients occurring over the narrow reaction zone. In this paper we are concerned with the numerical approximation of such smooth, but rapidly varying, functions, by the use of Chebyshev pseudo-spectral methods. Although reaction zones are, strictly speaking, not fronts, since the solution is typically infinitely differentiable across the reaction zone, we will use this term where appropriate to describe localized regions of rapid variation. We note that the problem of resolving functions with narrow layers occurs in other areas of application as well (e.g., wave propagation and solid mechanics).

In many applications there is only a single front associated with the solution. This typically occurs in combustion, for example, when the model accounts for only a single reaction. For such functions the use of a suitably chosen family of mappings, together with a Chebyshev pseudo-spectral approximation in the transformed coordinates, allows for a highly accurate approximation of the solution [4, 18]. However, in many applications the solution can exhibit multiple fronts. This can occur in combustion, for example, when a multiple reaction mechanism is necessary to adequately model the phenomena to be studied. In this case multiple fronts, not necessarily closely spaced, can occur. We note that other physical mechanisms can also lead to multiple fronts (e.g., [27]).

When there are multiple fronts the effectiveness of the adaptive pseudo-spectral method depends on the ability of the mapping family to resolve multiple regions of rapid variation. Many of the mappings employed in the computations can increase resolution within a specific region; however, their effectiveness can be degraded when employed to approximate multiple layers which are not closely spaced [7]. One alternative is to develop and employ mappings which can resolve multiple regions of rapid variation.

An alternative procedure is to employ multiple domains, chosen so that within each subdomain there is only a single region of rapid variation (layer). We note that multi-domain procedures may offer advantages over single domain procedures unrelated to the computation of problems with multiple layers. For example, (i) they are suitable for parallel computation, e.g., [11, 15], (ii) they may allow for more well-conditioned matrices, since within each subdomain a smaller number of collocation points can be used, and similarly, (iii) they may allow for larger timesteps for explicit schemes due to reduced spectral radii of the resulting differentiation matrices. Multi-domain procedures have been previously used to approximate functions with localized regions of rapid variation, e.g., [13, 21]; however, these calculations involved essentially one layer and the multi-domain procedure was employed to match a small inner region at the layer with larger domains away from the layer. The emphasis in this paper is on problems involving multiple layers, the adaptive determination of interface location, and the interaction of the domain decomposition with associated mappings within each subdomain. In particular, we will describe a procedure to determine interface locations adaptively from the locations of the layers, a problem which can be addressed in several ways. We will also demonstrate that points (ii) and (iii) above are not necessarily realized when approximating a function exhibiting layer type behavior, since in this case the condition number and spectral radius of the resulting differentiation matrices appear to depend upon the degree of expansion of the layer region due to the domain decomposition and the mapping, in addition to the number of collocation points employed.

The methods that we describe here will allow for adaptive, high resolution Chebyshev pseudo-spectral calculations of problems with multiple layers. We develop adaptive domain decomposition strategies in which subdomains are adaptively determined so that each subdomain contains only one layer. The methods we consider are based entirely upon the locations of the layers, so that adaptive determination of the locations of the layers automatically leads to adaptive determination of interface locations. We investigate two possible strategies relating interface location, layer location and the choice of mapping family and determine a preferred strategy based on numerical experiments approximating functions exhibiting layer-type behavior.

The problem of adaptive domain decomposition, in particular, adaptively determining interface locations, can then be reduced to the adaptive determination of layer location, a problem which has been extensively studied, particularly in the context of Chebyshev pseudo-spectral approximations. General techniques, involving the minimization of functionals monitoring the numerical error have been considered in [4, 5, 17, 18]. In these techniques the minimization must determine both the parameters of the mapping and the interface locations. Simpler techniques avoid the minimization problem by using properties of the differential equation, for example, by examining particular functions of the solution. In combustion, for example, estimates for the locations of the reaction zones can be obtained from the locations of the maxima of the reaction rate terms [11]. This procedure is employed in the numerical computations of a combustion model which we present here. We also compare different domain decomposition strategies by considering approximation of functions for which the locations of the layers are assumed known in advance.

Three considerations must be addressed in determining an adaptive multi-domain procedure, even assuming prior knowl-

edge of the layer location. These are: (i) to develop a procedure to adaptively determine the interfaces between adjacent subdomains, (ii) to determine a suitable family of mappings to employ within each subdomain, and (iii) to match the mappings to the interface determination strategy.

These points are related. In particular, the subdomains can be determined so that the layers are either interior to the subdomains, or are near the boundary. Depending upon the placement strategy, mappings can be used which are suitable for interior layers or boundary layers. We consider two possible domain decomposition strategies to resolve multiple layer solutions:

- Use an interior layer mapping and determine the domain interfaces so that the layer is located away from the boundary (strategy I (for interior)).
- Use a boundary layer mapping and determine the domain interfaces so that the layer is located at the boundary (strategy B (for boundary)).

We note that strategy I leads to one subdomain per layer while strategy B leads to two subdomains per layer. In Section 2 we describe the numerical method and the associated mappings. In Section 3 we describe the results of the two strategies when applied to the approximation of certain functions exhibiting two layer behavior. We also illustrate the domain decomposition method for a problem in combustion with multiple reactions.

2. NUMERICAL METHOD

We first describe the standard pseudo-spectral method. This description will be brief, since details can be found in [8, 10, 16]. For concreteness we consider a one-dimensional model equation

$$u_t = u_{xx} + R(u), \quad -1 \le x \le 1, \tag{1}$$

where $R(u)$ represents a nonlinear term not involving derivatives. We assume that the problem has been scaled to the interval I, $\{-1 \le x \le 1\}$. The solution is approximated by expanding u as a finite sum of Chebyshev polynomials

$$u \simeq u_J \equiv \sum_{j=0}^{J} a_j T_j(x). \tag{2}$$

In the pseudo-spectral method the expansion coefficients a_j are obtained from collocation; that is, the function u_J is forced to solve (1) at a set of $J + 1$ points x_j, called the collocation points. The unknowns of the problem are the values of u_J at the collocation points. Pseudo-spectral methods are particularly well suited to nonlinear problems because the nonlinearities are evaluated directly in terms of function values at the collocation points. The expansion (2) is used only for the purposes of computing spatial derivatives. Typically the collocation points are the Gauss–Lobatto points,

$$x_j = \cos(j\pi/J) \quad (j = 0, \ldots, J).$$

The major advantage of pseudo-spectral methods over finite difference methods is that they can exhibit enhanced accuracy for a fixed computational effort. In fact pseudo-spectral methods exhibit infinite-order accuracy. That is, the error $e = u - u_J$ satisfies, in an appropriate norm,

$$\|e\| = O(J^{-r}) \tag{3}$$

for all $r \ge 0$ and sufficiently differentiable functions u. The constants involved in the order relation in (3) depend upon the size of the derivatives of u. This is in contrast to finite difference methods where the error is of a fixed order, for example $O(J^{-2})$ for a second-order method. In practice spectral methods have been shown to be significantly more accurate than finite difference methods for a variety of problems in areas such as fluid dynamics and meteorology [8, 10, 16].

Pseudo-spectral methods are, however, prone to inaccuracies and oscillations when used to approximate functions with localized regions of rapid variation such as occur in many areas of application. In addition, there is evidence that these methods are significantly more accurate when the regions of rapid variation are located close to the boundaries, for example [7, 16, 28]. However, even boundary layers can exhibit oscillations if the layers are sufficiently thin.

One approach to enhance the accuracy of pseudo-spectral methods is to employ coordinate transformations so that in the transformed coordinate the function varies more gradually and so they can be better approximated by a polynomial expansion [1, 4, 5, 17, 18]. Specifically, assume that a family of mappings,

$$x = q(s, \boldsymbol{\alpha}), \tag{4}$$

is introduced. Here x represents the physical coordinate, $-1 \le s \le 1$ is the transformed coordinate, and $\boldsymbol{\alpha}$ denotes one or possibly more parameters to be determined in the course of the computation. The pseudo-spectral method can then be applied to the transformed equation to approximate the transformed function $u(q(s, \boldsymbol{\alpha}), t)$. The effect of the mapping can be regarded as transforming the function to be approximated to $u(q(s, \boldsymbol{\alpha}))$ from $u(x)$. If the mapping is properly chosen, for example, so that some measure of the approximation error is minimized, $u(q(s, \boldsymbol{\alpha}))$ will vary more gradually and so will be more readily approximated by a polynomial expansion.

The construction of a particular family of mappings is analogous to techniques in analysis, where thin layers are stretched by appropriate stretching factors so that the structure of the layer can be determined. In applications involving the numerical solution of partial differential equations, in particular in combustion, neither the location of the layer nor the appropriate degree of stretching is known in advance and must be obtained adaptively, i.e., from properties of the solution as it evolves in time. The adaptive procedure described in [4] employed a

functional which monitored the spectral interpolation error. Coordinate transformations were chosen which minimized the value of this functional. This approach can also be used to obtain interface locations [3].

It is also possible to use information from the underlying system of partial differential equations to determine appropriate mapping parameters. For example, in combustion, the locations of the reaction zones can be estimated from the maxima of the reaction rate terms, while the widths of the reaction zones can be estimated from a suitably nondimensionalized activation energy. In this way costly minimization problems can be avoided. This procedure is employed in our combustion calculations described.

In order to determine the most effective domain decomposition strategy, we also study the approximation of specific functions exhibiting layer-type behavior. We assume that the locations of the layers are known beforehand, as well as the widths of the layers. With the specification of layer locations and mapping parameters, the subdomain interfaces can be determined. In our approximation results, we present and compare strategies for adaptive domain decomposition for functions with multiple layers.

The effectiveness of the method depends on the properties of the family of mappings. Most families of mappings which have been used with this method are constructed so as to resolve a single region of rapid variation. The construction of families of mappings capable of resolving multiple regions of rapid variation would require additional parameters to characterize the family (i.e., the dimension of $\boldsymbol{\alpha}$ would become larger), thus resulting in a considerably more expensive minimization problem.

In applications it is generally known whether the layer to be resolved is an interior layer or a boundary layer, so that the particular family of mappings should be chosen to reflect this property. We have considered two families of mappings which have been employed as part of the adaptive pseudo-spectral method. The first family of mappings is a two-parameter family of mappings,

$$x = x_f + \tan((s - s_0)\eta)\alpha_I, \tag{5}$$

where s_0 and η are determined so that (5) maps the interval I onto itself. The values of s_0 and η, determined in this way are

$$s_0 = \frac{\nu - 1}{\nu + 1}, \quad \nu = \tan^{-1}(\alpha_I^{-1}(1 + x_f))/\tan^{-1}(\alpha_I^{-1}(1 - x_f)),$$

$$\eta = \tan^{-1}(\alpha_I^{-1}(1 - x_f))/(1 - s_0).$$

The parameters specifying each member of the family are x_f and α_I.

This mapping is chosen so that the q^{-1} is an approximation to a step function with a near discontinuity at $x = x_f$. The gradient of the inverse mapping near this point becomes larger as α_I decreases. Thus for those components of the solution that are close to step functions (in combustion these are typically temperature and concentration profiles) the result of the mapping is to get a transformed solution which is nearly linear and thus well approximated by a low order polynomial [7]. Thus α_I can be thought of as measuring the narrowness of the layer while x_f measures its location.

Although in principle the family of mappings (5) can also be applied to boundary layers, this requires the determination of two parameters and the mapping family becomes singular at $x_f = \pm 1$. A family of mappings designed to resolve boundary layers is

$$x = 4/\pi \tan^{-1}[\alpha_B \tan(\pi/4)(s - 1)] + 1, \tag{6}$$

which involves only one parameter. For $\alpha_B > 1$ the boundary near $x = -1$ is expanded while for $\alpha_B < 1$ the boundary near $x = 1$ is expanded. (We note that similar families of mappings can be constructed which expand the region around $x = 0$ at the expense of both boundaries. One such family was employed in [1, 2, 9] and allows for an arbitrary degree of expansion, while another family was employed in [20] and has the effect that the images of the Gauss–Lobatto points are nearly equally spaced.)

The mappings (5) and (6) can be effectively employed in a multiple domain computation if there is only one layer within each subdomain. The interval I is divided into one or more subdomains, which are then mapped to the interval I using a linear mapping. The solution is approximated within each subdomain using Chebyshev spectral or pseudo-spectral methods with appropriate interface conditions connecting the solution across the subdomain boundaries. Subdomains can be chosen so that within each subdomain the layer is a boundary layer or an interior layer. Once this choice is made the interfaces can be chosen adaptively from knowledge of the layer locations.

In the applications considered here we solve a problem of parabolic type. Appropriate interface conditions are continuity of the solution and its first derivative normal to the interface. We work in polar coordinates and take the interfaces as circles, so that the interface conditions are that u and u_r be continuous cross the interface, where u denotes any one of the dependent variables. We enforce these interface conditions by creating a differentiation matrix for the solution in the entire domain, i.e., encompassing all of the subdomains. The interface conditions are enforced by incorporating them directly into the differentiation matrix.

The use of multiple domains can lead to an improvement in accuracy by (i) resolving the thin layers in the problem by introducing domains corresponding to the length scales appropriate for the layers and (ii) isolating different regions of rapid variations so that each subdomain contains only one such layer and then employing mappings such as those described above to resolve the solution within the subdomains. The effectiveness of the method in resolving multiple layer problems depends

upon the choice of the subdomains and the mappings. A poor choice can lead to a significant degradation in accuracy [7].

When domain decomposition techniques are employed, the issue of boundary or interior layer becomes a crucial issue in designing the strategy to choose the locations of the subdomains. According to strategy B (boundary) the subdomains can be chosen so that within each subdomain the solution is a boundary layer. The advantages of the boundary layer approach are (i) Chebyshev approximations appear to be naturally more accurate for functions which vary rapidly near the boundary as opposed to functions which vary rapidly in the interior [7, 28] and (ii) only one parameter needs to be determined when the mapping family (6) is employed. A disadvantage is that the interface conditions, not the differential equations, are applied in the regions which are generally most nonlinear and most important for the overall solution (e.g., the reaction zones for combustion problems).

According to the alternative strategy, strategy I (interior), the subdomains are chosen so that the layers are located away from the boundaries. Within each subdomain the interior layer mapping (5) is employed, thus resulting in two mapping parameters which have to be determined (although the location of the layer can be determined by examining the reaction rate terms or other functions of the solution).

3. RESULTS

Our first numerical results are designed to compare strategies I and B in approximating functions exhibiting layer behavior. We therefore consider specified functions $f(x)$ defined for $-1 \leq x \leq 1$ exhibiting one or more layers. Both domain decomposition strategies require knowledge of the locations of the layers. In computations of partial differential equations, estimates of the locations of the layers would be obtained adaptively from the solution, as they are in our combustion calculations. In our approximation results, which are only designed to compare the two domain decomposition strategies, we assume that the locations of the layers are known.

Given knowledge of the layer locations, the interval $-1 \leq x \leq 1$ is decomposed according to the strategy considered. For strategy I the domains are chosen so that the layer is in the center and the interface between two layers is halfway between the layers. For strategy B the interface is at the center of the layer and the interface between two adjacent layers is in the center between the two layers. For each case we assume that the same number of points, N, is employed within each subdomain.

We next describe the different mappings that are applied within the subdomains. We let x denote the original coordinate. Each subdomain is first mapped to the interval $-1 \leq s' \leq 1$ via a linear mapping from x to a coordinate s'. A further mapping, of the form (5) for strategy I and (6) for strategy B is then applied within each subdomain. The Chebyshev interpolant to f is then computed as a function of s at the Gauss–Lobatto points. The accuracy of the approximation is then measured by computing the derivatives (in x) at the collocation points. Specifically we consider the errors

$$E_i = \max |d^i f/dx^i - D^i f|, \quad i = 1, 2,$$

where D denotes the differentiation operator on the collocation points for each multiple domain strategy and the maximum is taken over all collocation points. Similar results, although at lower error levels, are obtained for the approximation error; i.e., $i = 0$ with the error taken over different points other than the collocation points.

This procedure is designed to model the adaptive procedure proposed for the solution of partial differential equations. The main difference is that in the solution of partial differential equations the location of the layers is obtained from an adaptive procedure. In our combustion computations the layer locations can be determined from the maxima of the reaction rate terms. In addition, parameters for the layer mapping (either (5)) or (6) have to be determined. For both strategies I and B there is one mapping parameter, measuring the width of the region of rapid variation which has to be determined. We denote this parameter generically by α. Our approximation results are presented for those values of α for which the sum $E_1 + E_2$ is minimized.

We first consider the case of a single layer. In this case strategy I is simply a single domain computation employing the mapping (5). We note that this case has been analyzed in [7] for slightly different functions and error measures. We consider the function

$$f(x) = 1 - \tanh((x - s)/\varepsilon), \quad -1 \leq x \leq 1. \tag{7}$$

This function models the behavior of concentration profiles and, to some extent, temperature profiles for single reaction combustion models. There is a region of rapid variation at $x = s$, the width of which is proportional to ε.

The accuracy of the approximations using the two different strategies is compared for discretizations involving roughly the same computational effort in employing the approximations in solving partial differential equations. We assume that the pseudospectral method will be implemented using matrix multiplication to compute the spatial derivatives. In this case two domains with N_B points in each subdomain will require $O(2N_B^2)$ operations per timestep, while a single domain computation with N_I points will require $O(N_I^2)$ operations per timestep. Thus in order to have a comparable computational effort for each strategy N_I and N_B should be related by $N_I/N_B = \sqrt{2}$.

The location of the layer must be estimated for both strategies. The main feature of strategy B is that the interface location $'x_{INT}$ is taken as the location of the layer, while for strategy I the location of the layer is related to the parameter x_f in (5). In computations, estimates of the layer location can be obtained in general via minimization of functionals related to the approximation error [3, 4]. It is often possible, however, that this

TABLE I

Errors for Single Domain Approximation and Strategy B in Approximating $1 - \tanh((x - s)/\varepsilon)$

Strategy	s	α	N	E_1	E_2
I	0.0	.022	43	3.94×10^{-7}	1.38×10^{-4}
I	0.01	.014	43	5.52×10^{-5}	2.96×10^{-2}
B	0.0	.055	31	1.63×10^{-8}	3.35×10^{-5}
B	0.01	.045	31	6.38×10^{-6}	3.21×10^{-3}

minimization can be avoided and the layer location can be obtained by using properties of the differential equations. For example, in combustion problems the locations of the reaction zones can be obtained from the maxima of the reaction rate-terms. In the examples presented here we assume that the location of the layer is known via some technique and we focus on the accuracy of the two different strategies in approximating the solution.

An important consideration, however, is the effect of imperfect knowledge of the layer location. In applications the layer location may not be precisely known due to numerical errors associated with the procedure to determine layer location. In addition, there may be a cellular structure along the layer (e.g., along the front). In this case the layer location may vary with a coordinate along the front. In order to simplify both the transformations and the geometric domains, an average value of the layer location must be specified. In the examples presented here we test the sensitivity of the two strategies to variations in the layer location by varying s and fixing the location parameters $x_{\text{INT}} = x_f = 0$. We consider a variation in s of order of the thickness of the layer (ε) which corresponds to typical cells in our combustion computations. Deeper cells require more collocation points in order to use an interface which is independent of location along the front. In Table I we compare the errors for the two strategies for $\varepsilon = 1 \times 10^{-2}$. We note that problems in which the layer is located at the center of the domain represent the worst case for mappings such as (5) [7], so that improved results for this mapping might be expected for layer locations closer to the boundary.

The results in Table I indicate a marked improvement in accuracy for both first and second derivatives when the interface is located very close to the center of the layer (i.e., $s = 0$). These results reflect the tendency of Chebyshev approximations to better approximate boundary layers rather than interior layers, even when mappings are employed [7, 28]. When the interface is away from the layer location (i.e., $s = 0.01$) the accuracy of both methods is degraded. In this case as well the errors for strategy B are smaller than those for strategy I. However, this value of s is near the limit of accurate resolution for the second derivatives as the computed errors are very sensitive to small variations in N. Given the advantage of a multiple domain computation for parallel computation, the results indicate that a multiple domain approach employing strategy B may be more efficient than a single domain approach even for solutions exhibiting one layer.

We next consider a Gaussian function exhibiting spike-like behavior

$$f(x) = \exp(-((x - s)/\varepsilon)^2). \tag{8}$$

This models the behavior of the reaction rate terms typically occurring in combustion. We again set $x_l = x_f = 0$ and vary s in order to test the robustness of each strategy. Results comparing the single domain approximation with domain decomposition based on strategy B are given in Table II for $\varepsilon = 1 \times 10^{-2}$.

The results, while not as definitive as those in Table I demonstrate that strategy B is comparable to the single domain approximation and shows a definite superiority in approximating the first derivative when the interface location is near the layer location. As before, the accuracy of the approximation degrades when s is of the order of ε.

We have examined the condition numbers of the differentiation matrices in the original coordinate, which includes the derivative of the mapping, produced by both strategies. We find little differences in the spectral radius for the differentiation matrices produced by strategy B over one subdomain and that produced by strategy I over the full domain. Indeed, the spectral radius for the first derivative matrix for the case corresponding to the first entry in Table I is 714, while for the third entry (two domain calculation) it is 1148. Analogous numbers for the second derivative matrix are 5.09×10^5 and 6.95×10^5. Thus the spectral radius for the single domain with 43 points is smaller than that for the subdomain with 31 points. Examination of the resulting collocation points indicates that the strategy B approximation results in a greater clustering of collocation points in the layer than for strategy I. We believe that this accounts for the reduced spectral radius for the strategy I approximation even though the number of collocation points is greater. We conclude that when domain decomposition methods are employed to resolve problems with layers, the spectral radius depends most critically on the clustering of collocation points within the layer, which is related to the resolution of the layer, rather than the particular domain decomposition strategy.

TABLE II

Errors for Single Domain Approximation and Strategy B in Approximating $\exp(-((x - s)/\varepsilon)^2)$

Strategy	s	α	N	E_1	E_2
I	0.0	.030	43	1.65×10^{-4}	1.57×10^{-2}
I	0.01	.028	43	8.82×10^{-4}	$1.01 \times 10^{+0}$
B	0.0	.055	31	1.38×10^{-5}	1.94×10^{-2}
B	0.01	.080	31	2.01×10^{-3}	3.09×10^{-1}

TABLE III

Errors for Strategies B and I in Approximating
$(2 - \tanh((x - s_1)/\varepsilon) - \tanh((x - s_2)/\varepsilon))/2$

Strategy	s_1	s_2	α	N	E_1	E_2
I	0.5	−0.5	.037	43	2.00×10^{-7}	3.69×10^{-5}
I	0.49	−0.49	.028	43	1.31×10^{-5}	1.20×10^{-3}
B	0.5	−0.5	.100	31	7.07×10^{-9}	1.20×10^{-5}
B	0.49	−0.49	.095	31	3.20×10^{-6}	1.84×10^{-3}

We next consider the approximation of functions exhibiting a multiple layer structure. We first consider the function

$$f(x) = (2 - \tanh((x - s_1)/\varepsilon) - \tanh((x - s_2)/\varepsilon))/2, \quad -1 \le x \le 1, \tag{9}$$

with $\varepsilon = 1 \times 10^{-2}$. This function exhibits two layers, at $x = s_1$ and $x = s_2$, respectively. In order to test the robustness of the methods we consider the values $s_1 = -s_2 = 0.5$ as well as perturbations of these values. As before we consider the location parameters to be known. Thus for strategy I we use two subdomains, DI_1: $-1 \le x \le 0$ and DI_2: $0 \le x \le 1$ with the location parameter of the mapping $x_f = 0$ in each subdomain. For strategy B we employ four subdomains DB_1: $-1 \le x \le -0.5$, DB_2: $-0.5 \le x \le 0$, DB_3: $0 \le x \le 0.5$, and DB_4: $0.5 \le x \le 1$. We test the robustness of each strategy by varying s_1 and s_2. The robustness of both methods to variations in the layer locations is tested by varying s_1 and s_2. As each subdomain is mapped to the interval I by a linear mapping, differences between the layer location and the interface location or the location parameter x_f may be magnified after this mapping is applied. This factor should be considered in assessing resolution requirements for problems with multiple layers. The two strategies are compared in Table III.

The results demonstrate again that strategy B is preferable when the interfaces are near the layer locations. The errors for strategy B are reduced from those of strategy I by approximately a factor of 5 for the first derivatives and by about a factor of 2 for the second derivatives. Both methods degrade as the interfaces move away from the layer location. Strategy B leads to nearly an order of magnitude reduction for the error in the first derivatives, although for this particular case, the error for the second derivative is somewhat larger than for strategy I.

Finally we consider the approximation of a function exhibiting multiple spikes by considering the function

$$f(x) = (\exp(-((x - s_1)/\varepsilon)^2) + \exp(-((x - s_2)/\varepsilon)^2))/2. \tag{10}$$

Results comparing the two strategies for $s_1 = -s_2 = \frac{1}{2}$ are given in Table IV.

The results for all four test cases are consistent with previous studies of the effect of layer location on the accuracy of Chebyshev approximation for functions with narrow regions of rapid variation. There is a tendency for Chebyshev pseudo-spectral methods to provide more accurate approximations for boundary layers as opposed to interior layers, e.g., [7, 28]. Indeed, the direct Chebyshev approximation of interior layers (i.e., without mappings) is a difficult problem requiring a large number of collocation points. It is shown in [7] that the mapping (5) makes possible the efficient approximation of both interior and boundary layers, provided the parameters of the mapping are properly chosen. The use of mappings such as (5) reduces, but does not eliminate, the disparity in accuracy in the approximation of boundary layers as opposed to interior layers. This explains the results presented here, which show that strategy B allows a more efficient approximation of multiple layers than strategy I and is thus a preferred method for adaptive domain decomposition. This difference is persistent over a range of functions and examples beyond those presented here.

A potential question associated with strategy B, however, is the effect of imposing interface conditions rather than the differential equations at points within the layer, rather than away from the layer. For example, in combustion the interface conditions would be imposed in the reaction zone, where the chemical reaction terms are most important and are extremely sensitive to the pointwise value of the temperature, rather than away from the reaction zone, where the solution varies gradually, as in strategy I. It can be shown that domain decomposition approximations maintain spectral accuracy [10]. However, imposition of the interface conditions at points where the solution varies rapidly can possibly lead to large numerical errors. This is an effect which cannot readily be analyzed by examining the approximation of given functions. We illustrate that this does not lead to significant errors by direct implementation of strategy B in the solution of partial differential equations governing combustion with a sequential reaction mechanism.

We consider the diffusional thermal model for combustion with a sequential reaction mechanism. The reaction mechanism is described schematically by

$$A \to \mu B \to C, \tag{11}$$

where μ is the stoichiometric coefficient for the first reaction.

TABLE IV

Errors for Strategies B and I in Approximating
$(\exp(-((x - s_1)/\varepsilon)^2) + \exp(-((x - s_2)/\varepsilon)^2))/2$

Strategy	s_1	s_2	α	N	E_1	E_2
I	0.5	−0.5	.061	43	5.63×10^{-5}	1.04×10^{-2}
I	0.49	−0.49	.067	43	3.32×10^{-3}	3.46×10^{-1}
B	0.5	−0.5	.105	31	1.28×10^{-5}	3.84×10^{-3}
B	0.49	−0.49	.130	31	8.80×10^{-4}	1.24×10^{-1}

Thus reactant A is converted to an intermediate species B prior to being converted to the final product C. Although this mechanism is itself highly simplified and, in practice, many reactions will occur in the combustion of even the simplest mixtures, reaction models of the form (11) have been used with considerable success in modeling the combustion of hydrocarbons; see e.g., [12, 29] (the intermediate is then CO and the final product is CO_2).

We assume that species A is deficient relative to the other species in the reacting mixture so that changes in the concentrations of the other species need not be tracked. After a suitable nondimensionalization (see [25, 26]) the equations of the diffusional thermal model become

$$Y_t = \nabla^2 Y/L_y - \mathbf{V}\cdot\nabla Y - \beta^2\Lambda Y W_1, \tag{12}$$

$$Z_t = \nabla^2 Z/L_z - \mathbf{V}\cdot\nabla Z + \beta^2\Lambda(YW_1 - ZKW_2), \tag{13}$$

$$\Theta_t = \nabla^2\Theta - \mathbf{V}\cdot\nabla\Theta + \beta^2\Lambda(\delta YW_1 + (1-\delta)ZKW_2), \tag{14}$$

where W_1 and W_2 are the nondimensional Arrhenius reaction rate terms for the two reactions (the expressions are given in detail in [26]), L_y and L_z are the Lewis numbers (ratio of thermal to mass diffusivity) for species A and B, respectively, Θ is a suitably nondimensionalized temperature so that $\Theta = 1$ corresponds to the adiabatic burned temperature of the mixture and $\Theta = 0$ corresponds to the temperature of the fresh mixture, and Y and Z are the mass fractions of species A and B, respectively. Λ, β, and δ depend on the physicochemical parameters of the problem.

Equations (12)–(14) describe the diffusion of mass and heat, the advection of the mixture due to the gas velocity V, and the chemical reaction. In our model we consider the case of a cylindrical flame stabilized by a line source of fuel of strength $2\pi\kappa$ so that

$$\mathbf{V} = \frac{\kappa}{r}\hat{\mathbf{r}},$$

and we solve (12)–(14) in polar coordinates r and ψ. The linear stability analyses in [25, 26] suggest parameter regimes in which axisymmetric flames are to be expected as well as parameter regimes in which cells along the flame front are to be expected.

The boundary conditions are

$$\Theta \to 1, \quad Y, Z \to 0 \quad \text{as } r \to \infty, \tag{15}$$

and

$$\Theta, Z \to 0, \quad Y \to 1 \quad \text{as } r \to 0. \tag{16}$$

Since the solutions are nearly constant for r large or for r near 0, these boundary conditions are imposed at finite, nonzero points, r_∞, and r_0 which are far from the reaction zones. We have verified that the solutions we have computed are insensitive to the locations of these points. We have implemented a domain decomposition method based on strategy B to compute the solutions to (12)–(14). We have computed both axisymmetric and cellular flames.

We employ a Fourier pseudo-spectral method in ψ and a Chebyshev multi-domain method in r. The domain interfaces are chosen to be circles so that the interface conditions are that all variables and their radial derivatives are continuous across the interfaces. We construct a single differentiation matrix over the entire domain in r. The interface conditions are incorporated directly into the matrix. The temporal integrator is a semi-implicit scheme consisting of backward Euler on the diffusive terms and forward Euler on the advective and reaction terms. In the backward Euler step approximate factorization is employed to allow for matrix inversion separately in the r direction and the ψ direction. A detailed description of the temporal integrator is given in [6].

We have implemented a domain decomposition method based on strategy B to compute the solutions to (12)–(14). We first consider the one-dimensional (axially symmetric) case. In our computations the domain interfaces are determined adaptively during the course of the computation by determining the maximum of the reaction rate terms YW_1 and ZW_2 in (12)–(14). Strategy B is implemented by locating the points at which the reaction rates attain their maxima. Call these points r_Y and r_Z, respectively. With these points determined adaptively we now have three subdomains $D_1 = [r_0, R_Y]$, $D_2 = [r_Y, r_Z]$, and $D_3 = [r_Z, r_\infty]$ and the solution within these subdomains is expected to exhibit boundary layer behavior at the interface points r_Y and r_Z. We further split D_2 into two subdomains, since the solution is expected to exhibit boundary layer behavior at both ends of this subdomain and our method is based on the assumption of one layer per subdomain. Thus defining $r_M = (r_Y + r_Z)/2$, we have two inner domains $D_{21} = [r_Y, r_M]$ and $D_{22} = [r_M, r_Z]$ in the flame.

We have computed a stationary, axisymmetric stready state to (12)–(14) for the parameters

$$\beta = 10, \quad L_y = 0.5, \quad L_x = 0.4, \quad \kappa = 25., \quad \delta = 0.5$$

We employed four domains, constructed as described above, with 25 points within each subdomain.

These parameters give rise to a well-separated flame. In Fig. 1 we plot Θ, Y, and Z for the steady state solution while in Fig. 2 we plot the reaction rate terms YW_1 and ZW_2. This solution has been validated by grid refinement. The results indicate that accurate solutions to partial differential equations can be obtained using strategy B, and in particular the maxima of the reaction rate terms provide an effective adaptive procedure to determine the interfaces. There does not seem to be any significant error in imposing the interface conditions in the reaction zone.

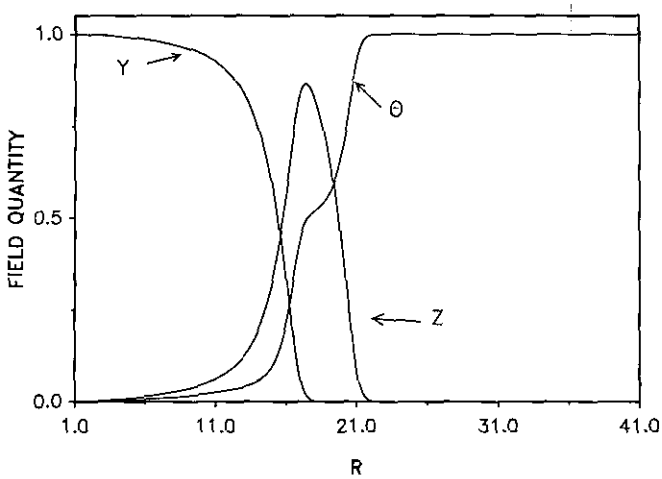

FIG. 1. Θ, Y, Z for stationary axisymmetric flame.

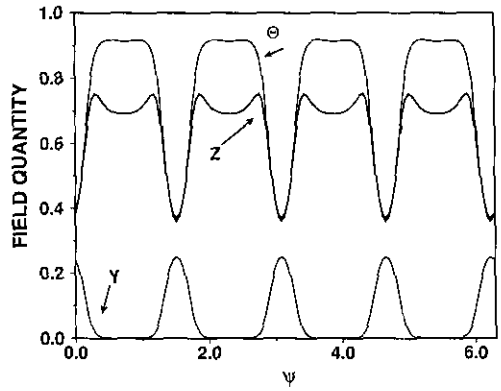

FIG. 3. Angular dependence of Θ, Y, and Z for a cellular flame with sequential reaction mechanism. Parameters are given in the text.

We have also used this method to compute cellular sequential flames, in which the unknowns exhibit a periodic dependence on the polar angle ψ. For nonaxisymmetric calculations the locations of the reaction zones vary with the angle ψ. Therefore the locations of the maxima for the reaction terms, r_Y and r_Z vary with ψ as well. In order to keep the interfaces geometrically simple, we average the reaction terms over all angles, then find the maxima in r, and use these maxima to determine the interfaces between adjacent subdomains. This procedure is similar to that employed in single domain calculations, e.g., [6], where the mapping parameters are chosen independent of ψ.

In Fig. 3 we plot Θ, Y, and Z as a function of ψ for a stationary four-cell solution. The parameters of the calculation are

$$\beta = 7.7, \quad \sigma = 1.051, \quad L_y = 0.37, \quad L_x = 0.9,$$

$$\delta = 0.85 \quad \kappa = 14.8, \quad \gamma = 0.385, \quad b = 1.$$

We note that the intermediate Z exhibits a different angular behavior from Θ or Y. Both Θ and Y exhibit behavior characteristic of a four cell, with four distinct minima and maxima for $0 \le \psi \le 2\pi$. The intermediate Z exhibits eight distinct maxima. As ψ varies the intermediate is consumed over regions of high temperatures; however, Z also attains minima at temperature minima where there has not been sufficient conversion of A into B. Thus Z attains its maxima at values of Θ in between the maximum and minimum temperatures. There are two such points per cell, thus resulting in the double peak cellular structure indicated in the figure.

In Fig. 4 we plot the loci of the maxima of the reaction rate terms, which characterize the two reaction zones and which are employed in the adaptive domain decomposition procedure. There are two curves, the inner curve is associated with the formation of the intermediate species while the outer curve is

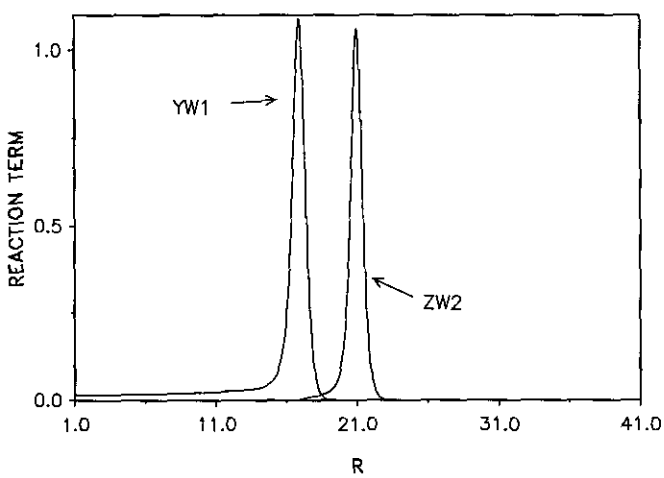

FIG. 2. Reaction rate terms for same flame as in Fig. 1.

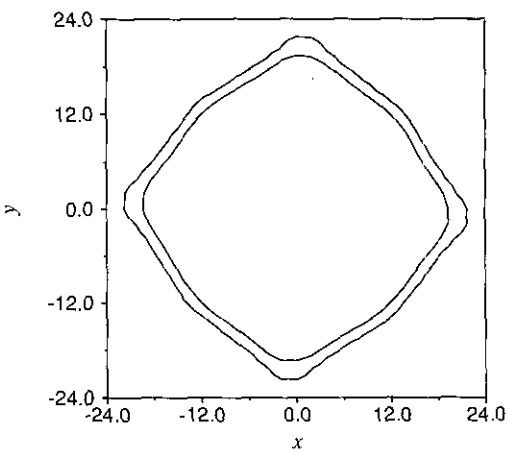

FIG. 4. Loci of the maxima of the reaction rate terms for a cellular flame with sequential reaction mechanism. Parameters are given in the text.

associated with the burning of the intermediate species. The cellular structure of the reaction zone is clearly visible, particularly for the second reaction. In interpreting this picture, note that the fresh mixture emanates from a point source at the center of the domain. The crests (at roughly 0°, 90°, 180°, and 270°) therefore point in the direction of the burned gases. There are no significant differences in the solution when the number of collocation points is increased.

REFERENCES

1. J. Augenbaum, *Appl. Numer. Math.* **5,** 459 (1989).
2. A. Bayliss, *J. Sound Vibr.* **60,** 543 (1978).
3. A. Bayliss, T. Belytschko, D. Hansen, and E. Turkel, in *Proceedings, 5th SIAM Conference on Domain Decomposition Methods for Partial Differential Equations,* edited by Keyes, Chan, Meurant, Scroggs, and Voigt (SIAM, Philadelphia, 1992), p. 195.
4. A. Bayliss, D. Gottlieb, B. J. Matkowsky, and M. Minkoff, *J. Comput. Phys.* **81,** 421 (1989).
5. A. Bayliss and B. J. Matkowsky, *J. Comput. Phys.* **71,** 147 (1987).
6. A. Bayliss, B. J. Matkowsky, and H. Riecke, *Physica D* **74,** 1 (1994).
7. A. Bayliss and E. Turkel, *J. Comput. Phys.* **101,** 349 (1992).
8. J. P. Boyd, *Chebyshev & Fourier Spectral Methods,* Lecture Notes in Engineering, Vol. 49 (Springer-Verlag, New York, 1989).
9. J. P. Boyd, *J. Comput. Phys.* **98,** 181 (1992).
10. C. Canuto, M. Y. Hussaini, A. Quarteroni, and T. A. Zang, *Spectral Methods in Fluid Dynamics* (Springer-Verlag, New York, 1987).
11. F. Desprez and M. Garbey, in *Proceedings, Parallel CFD 93,* to appear.
12. F. L. Dryer and I. Glassman, in *Fourteenth Symposium (International) on Combustion* (The Combustion Institute, Pittsburgh, 1972), p. 987.
13. U. Ehrenstein, H. Guillard, and R. Peyret, *Int. J. Numer. Methods Fluids* **9,** 499 (1989).
14. M. Garbey, in *Proceedings of 5th SIAM Conference on Domain Decomposition Methods for Partial Differential Equations,* edited by Keyes, Chan, Meurant, Scroggs, and Voigt (SIAM, Philadelphia, 1992), p. 293.
15. D. Gottlieb and R. S. Hirsh, *J. Sci. Comput.* **6,** 309 (1989).
16. D. Gottlieb and S. A. Orszag, *Numerical Analysis of Spectral Methods: Theory and Applications,* C.B.M.S.-N.S.F. Conference Series in Applied Mathematics (SIAM, Philadelphia, 1977).
17. H. Guillard, J. M. Male, and R. Peyret, *J. Comput. Phys.* **102,** 114 (1992).
18. H. Guillard and R. Peyret, *Comput. Methods Appl. Mech. Engrg.* **66,** 17 (1988).
19. D. Hansen, M.S. dissertation, Dept. of Electrical Engineering and Computer Science, Northwestern University, 1990 (unpublished).
20. D. Kosloff and H. Tal-Ezer, *J. Comput. Phys.* **104,** 457 (1993).
21. M. G. Macareg and C. L. Street, *Appl. Numer. Math.* **2,** 95 (1986).
22. S. B. Margolis and B. J. Matkowsky, *Combust. Sci. Technol.* **27,** 193 (1982).
23. B. J. Matkowsky, L. J. Putnick, and G. I. Sivashinsky, *SIAM J. Appl. Math.* **38,** 489 (1980).
24. B. J. Matkowsky and G. I. Sivashinsky, *SIAM J. Appl. Math.* **35,** 230 (1978).
25. J. Pelaez and A. Linan, *SIAM J. Appl. Math.* **45,** 503 (1985).
26. J. Pelaez, *SIAM J. Appl. Math.* **47,** 781 (1987).
27. K. G. Shkadinsky, G. V. Shkadinskaya, B. J. Matkowsky, and V. A. Volpert, *SIAM J. Appl. Math.* **53,** 128 (1993).
28. A. Solomonoff and E. Turkel, *J. Comput. Phys.* **81,** 239 (1989).
29. C. K. Westbrook and F. L. Dryer, *Combust. Sci. Technol.* **27,** 31 (1981).